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A Fortran Program for Analysis of Ellipsometer Measurements

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A general Fortran program is given that performs
the calculations required to analyze ellipsometer
measurements. This program replaces the program given
in NBS Technical Note 242, entitled "A Fortran Program
for Analysis of Ellipsometer Measurements and Calcula-
tion of Reflection Coefficients From Thin Films." The
main changes from the previous program are: 1) the
new program is in Fortran IV and V rather than Fortran
II; 2) the relative transmission of the wave plate is
considered in analyzing ellipsometer readings; 3) an
improved method is used for calculating the refractive
index of a film; 4) the form of the input data is
improved; 5) a method for calculating and correcting
for tilt of the reflecting surface is given; 6) an
improved method of calculating confidence limits for
the calculated values of thickness and refractive
index of a film is used; and 7) a method for calcu-
lating the optical constants of an adsorbing film of
given thickness is included.

Key words: Computer programs; ellipsometry; Fortran
program; multiple films; optical constants; reflection
coefficients; thin films.

1. Introduction

The reflection of polarized light from surfaces and thin films

has been discussed by various authors [1-4].* The reflection is

expressed in terms of the reflection coefficients R^p for light

polarized parallel to the plane of incidence and R^s for light

polarized perpendicular to the plane of incidence. Since these

coefficients are complex quantities, they represent both the change

of amplitude and phase of the light on reflection.

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*Figures in brackets indicate the literature references on page 62.

The ellipsometer is an optical instrument used to study surfaces and surface films by reflection of light from the surface. The ellipsometer measures the ratio of the reflection coefficients

$$\rho = R^p/R^s = \tan\psi \; e^{i\Delta}. \tag{1}$$

In the ellipsometer, as considered by this program, monochromatic light passes through a polarizer and a wave plate (linear retarder). It is then reflected from the surface under investigation, and passes through another polarizing prism called an analyzer and to a detector. The wave plate is generally set at a fixed azimuth and the polarizer and analyzer rotated until the light is extinguished as determined by the detector. The azimuths of the polarizer, fast axis of the wave plate, and analyzer, (P, Q, and A), measured from the plane of incidence are recorded. From the reading P, Q, and A, Δ and ψ of eq (1) are first calculated, then the optical constants of the surface or of films on the surface are calculated from Δ and ψ.

In order to calculate Δ and ψ from the ellipsometer readings, the constants of the wave plate must be known. Until recently, the relative phase retardance, Δ_c, along the fast and slow axes was believed to describe the optical properties of the wave plate. However, it has been shown [5-8] that the transmissions along the two axes are different. Therefore, the ratio T_c of the transmission along the fast axis to the transmission along the slow axis of the wave plate must also be considered. In addition, Oldham [6] has shown that a tilt in the mounting of the wave plate can cause Δ_c and T_c to vary with the azimuth of the wave plate. This program takes both Δ_c and T_c and their variation with Q into consideration in computing Δ and ψ. The values of Δ_c and T_c may also be computed from the ellipsometer readings.

Another possible source of error is a tilt of the reflecting surface. The instrument is alined so that P, Q, and A are read with respect to the reflecting surface. If the reflecting surface is changed, and the new surface is tilted with respect to the

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surface with which the ellipsometer was aligned, the readings of P, Q, and A will be in error. This error could be eliminated by re-alinement, but this is time consuming. Therefore, the program has been written to calculate the angle of tilt from the ellipsometer readings and correct for the tilt.

2. Data Input Required for Calculations

The data and instructions are given to the computer by punched cards. Each card requires an instruction starting in column 1. The data required for the instruction start in columns 10, 20, 30, 40, 50, and 60. All numbers must contain a decimal point.

Instructions that start with C cause the computer to perform calculations. These instructions are listed in table 1. The other instructions are used to give data for future calculations. Table 2 gives the required data with each instruction.

2.1. Table of Values for Δ, ψ, P, A, and Reflection Coefficients for a Film-Covered Surface - CTABLE

The instruction CTABLE will produce calculation of ellipsometer readings and reflection coefficients for reflection of light from a film-covered surface. The thickness of the film is given on the same card as the instruction. However, before the CTABLE instruction is given, instructions NM, NF, NS or CNS, AI, and WL (see table 2) must be used to give values of the refractive index of the medium, film, and substrate and the angle of incidence and wave length of the light, respectively. For example,

1	10	20	30	40
NM	1.			
NF	1.4			
NS	1.7			
AI	65.			
WL	4800.			
CTABLE	40.			

Table 1. Computations

Instruction	Computes	Preceding Instructions Required If Standard Values Are Not Used
CAT	Angle of tilt of reflecting surface	WP or CWP
CD	Thickness of film	NM, NF, NS or CNS, AI, NREF, WL[1]
CND	Refractive index and thickness of film	NM, NF, NS or CNS, AI, NREF, WL, ELDP[1]
CNDC	Refractive index and thickness of film with allowed combination of values	NM, NF, NS or CNS, AI, NREF, WL, ELDP, EDP[1]
CNDE	Refractive index and thickness of film with confidence limits	NM, NF, NS or CNS, AI, NREF, WL, ELDP, EDP[1]
CNK	Refractive index and $\varkappa$ of film of given thickness	NM, NF, NS or CNS, AI, NREF, WL, FT[1]
CNS	Refractive index of substrate	NM, AI, NREF[1]
CTABLE	Table of Δ and ψ and reflection coefficients	NM, NF, NS or CNS, AI, NREF, WL
CWP	Constants T_c and Δ_c of wave plate	None

[1] Instructions WP or CWP required if ellipsometer readings (P, A, and Q) are given.

Table 2. Data Given With Instructions

Card Column No.

1	10	20*	30	40	50*	60
AI	$I(\varphi)$	$\delta(\varphi)$	$E(\varphi)$			
ALINE	ΔP	ΔA	ΔQ			
AT	Angle					
CAT	P_1	A_1	P_2	A_2	Q	
CATA	P_1	A_1	P_2	A_2	Q	
CD						
CND	Δ	ψ				
CNDC	P	A	Q			
CNDE	P_1	A_1	P_2	A_2	Q	
CNK	blank					
CNS						
CTABLE	$I(d)$	$\delta(d)$	$E(d)$	Q**		
CWP	P_1	A_1	P_2	A_2	Q	
EDP	$E\Delta$	$E\psi$				
ELDP	$EL\Delta$	$EL\psi$				
FILM	No.	d	n	$\varkappa$		
FT	$I(d)$	$\delta(d)$	$E(d)$			
IFILM	No. films	d	n_{top}	$\varkappa_{top}$	n_{bottom}	$\varkappa_{bottom}$
MIXED	ρ_1	ρ_p	n_p			
NF	$I(n)$	$\delta(n)$	$E(n)$	$I(\varkappa)$	$\delta(\varkappa)$	$E(\varkappa)$
NM	$I(n)$	$\delta(n)$	$E(n)$			
NREP	No. Reflections					
NS	$I(n)$	$\delta(n)$	$E(n)$	$I(\varkappa)$	$\delta(\varkappa)$	$E(\varkappa)$
PAGE	See Section 2.12					
RESET	See Section 2.12					
STØP						
WL	$I(\lambda)$	$\delta(\lambda)$	$E(\lambda)$			
WP	T_c	Δ_c				
(other)	Comment					

* The symbol δ refers to incremental values.

**The value of Q with this instruction is optional. See Section 2.1.

Table 3. Assigned Values

Symbol	Data	Instruction	Assigned Values
N_n	Index of medium	NM	1
N_2	Index of film	NF	1
N_s	Index of substrate	NS	1
φ_1	Angle of incidence	AI	70°
λ	Vacuum wavelength of light	WL	5461
T_c, Δ_c	Constants of wave plate	WP	1, 90°
	Number of reflections of light	NREF	1
	Experimental errors of Δ and ψ	EDP	.015, .015
	Error limits of Δ and ψ used for computing n_2	ELDP	.002, .002
	Angle of tilt	AT	0

will compute Δ and ψ and reflection coefficients for the condition:

Refractive index of medium   = 1.
Wave length of light   = 4800. Å
Angle of incidence   = 65.°
Thickness of film   = 40. Å
Refractive index of film   = 1.4
Refractive index of substrate = 1.7

A range of values of the input parameters may also be speci-
fied by giving the initial value, increment, and final value to be
used. Thus, the input data

1	10	20	30	40
NM	1.			
NF	1.4	0.1	1.6	
NS	1.7			
AI	65.			
CTABLE	0.	20.	100.	

will produce tables for films of refractive index of 1.4, 1.5, and
1.6. In each table, the ellipsometer readings and reflection
coefficients will be given for films 0, 20, 40, 60, 80, and 100 Å
thick. The results are given in the upper portion of figure 1.
The other parameters may also be similarly varied.

In this figure the values of Δ and ψ for the sample, then the
complex reflection coefficients for light polarized parallel and
normal to the plane of incidence, are printed. For the complex
reflection coefficients, the ratios of reflected to incident ampli-
tudes and the change in degrees of the phase of the light are given.
The intensity ratios for parallel and normally polarized light are
the squares of the corresponding amplitude ratios.

The refractive index and value of n for the film and substrate
are next printed. In this example, the film and substrate are non-
absorbing so the values of n are zero.

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A setting, Q, for the wave plate starting in column 40, may also be given with the CTABLE instructions. In this case, the two sets of ellipsometer readings, P1,A1 and P2,A2, (see Section 2.3) that will produce extinction of the light are also calculated and printed, as shown in figure 1.

Listed in table 3 are values for certain of the input parameters. These assigned values are automatically used for following calculations unless instructions are given to change them. Thus, in the above examples, the NM instruction was not necessary as the assigned value of 1. was used for the index of the medium.

The film or substrate may also be absorbing. In this case the optical constants are n and $\varkappa$ of the complex refractive index $n - n\varkappa i$. The values of n and $\varkappa$ are given starting in columns 10 and 40. Thus, the card

<div align="center">Column No.</div>

1	10	20	30	40
NS	3.316			1.4

defines an absorbing substrate with n=3.316 and $\varkappa$=1.4 or of complex refractive index of 3.316(1-1.4i).

The value of n may be varied by giving the initial, incremental, and final values starting in columns 10, 20, and 30, and $\varkappa$ may be varied by giving the initial, incremental, and final values starting in columns 40, 50, and 60.

2.2. Optical Constants of a Film-Free Substrate - CNS

The instruction CNS calculates the optical constants n_s and $\varkappa_s$ of a substrate from measurements of Δ and ψ for the substrate without a film. The values of Δ and ψ start in columns 10 and 20 of the card containing CNS. The values of n_s and $\varkappa_s$ are printed and also retained by the computer so they will be used in following calculations, such as CTABLE, for which they are required. Thus, the optical constants of the substrate may be given by either an NS or CNS instruction.

Ellipsometer readings of P, A, and Q, rather than values of Δ and ψ may be used with the CNS instruction, as explained in the next section.

2.3. Input of Ellipsometer Readings P, A, and Q

As previously described, the ellipsometer readings must first be analyzed to obtain the values of Δ and ψ that describe the reflection of the light from the surface before the instruction CNS, or the instructions CD, CND, CNDC, CNDE to be later described, may be used. However, the ellipsometer readings may also be used as input data with these instructions if the components of the ellipsometer are arranged in the order of light source, polarizer, wave plate, reflecting surface, analyzer, and detector.

Let the wave plate be set with its fast axis at an azimuth Q and let extinction of the light be obtained with the polarizer and analyzer at azimuths P and A (see Reference 4). All azimuthal angles are measured positive counterclockwise from the plane of incidence. Then these readings of P, A, and Q may be used with the above instructions, as shown in table 2. The computer first calculates the values of Δ and ψ and uses them in the following calculations.

Let P_1 and A_1 be settings of the polarizer and analyzer that produce extinction of the light for a given value of Q. Then, settings of for example P_1 + 180°, A_1 ; P_1, A_1 + 180°; and P_1 + 180°, A_1 + 180° produce the same effect on the polarized light so will also give extinction. That is, P and A are indeterminate to ±180°. This duplication of settings may be eliminated by, for example, taking only P and A readings between 0 and 180°. After eliminating duplicate readings, two sets of readings P_1,A_1 and P_2,A_2 will be found to give extinction for a given setting Q of the wave plate. Both sets of readings may be used with the instructions CD, CND, CNDE, and CNS. They are given in the order P_1, A_1, P_2, A_2, Q.

The computer calculates values of Δ and ψ from each set of readings and uses the averages of them in the following calculations.

In order for the computer to calculate Δ and ψ from the ellipsometer readings, the constants of the wave plate must have been previously made available to the computer. The constants are the ratio, T_c , of the transmittance of the wave plate along the fast axis to the transmittance along the slow axis and the phase retardance along the fast axis minus the phase retardance along the slow axis, Δ_c . They may be given in the order T_c , Δ_c with the instruction WP or may be calculated from a set of readings P_1, A_1, P_2, A_2 and Q by the CWP instruction.

More than one calculation may be performed with a single set of ellipsometer readings. In this case, a set of ellipsometer readings from a film-free metal surface is used to first calculate the constants of the wave plate by the CWP instruction, and then is used to calculate the optical constants of the metal by the CNS instruction. The readings do not have to be repeated with the CNS instruction.

2.4. Corrections to Ellipsometer Readings: ALINE, AT, CAT, CATA

The ellipsometer angular readings of P, A, and Q must sometimes be corrected to obtain angles measured from the plane of incidence of the reflection from the surface, as is required for this program. For example, if a dial reads from the plane of the surface, 90° must be added to the dial readings. As another example, in alining the ellipsometer the dial readings when the component is alined in the plane of incidence may be recorded and used as a correction to future readings of the dial, rather than adjusting the dial or the vernier on the dial to read correctly. This method of alinement is described in Appendix I.

The corrections (ΔP, ΔA, and ΔQ) may be given by the ALINE Instruction (see table 2). Then the corrections will be added to values of P, A, and Q given with all following instructions.

A correction to the ellipsometer readings may also be required due to tilting of the reflecting surface. This may occur when the ellipsometer is alined with one surface, and then the surface is replaced by another surface that is to be measured. The second surface may be tilted with respect to the orientation of the first surface so the ellipsometer will no longer be properly alined but all its readings must be corrected by the angle of tilt. This correction may be given to the computer by the AT instruction. The AT instruction differs from the ALINE instruction in that one correction is given to be added to all values of P, A, and Q, while different corrections for P, A, and Q are given with the ALINE instruction.

The angle of tilt of the reflecting surface is generally unknown. It may be computed from ellipsometer readings by the instruction CAT. The instruction CAT requires the two sets of P and A readings for a setting of Q and the constants T_c and Δ_c of the wave plate. The calculated value of the angle of tilt will be added to all ellipsometer readings given by following instructions.

The theory of this calculation is given in Section 3.3. This theory requires that the angle of tilt is small. The calculation has been found to be accurate for angles of tilt up to one degree.

The constants of the wave plate may not be calculated from the same readings used to compute the angle of tilt, since readings from an untilted surface are required to compute the wave plate constants. The usual procedure is to aline the ellipsometer and calculate the constants of the wave plate from ellipsometer readings. Then, every time the surface is changed, its angle of tilt is calculated using the previously determined constants of the wave plate. The angle of tilt of the surface is then used to correct all ellipsometer readings obtained using the surface.

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Often two sets of ellipsometer readings are taken for the same surface. For example, readings may be taken for two readings of Q or readings may be taken both before and after a film forms on the surface. Values for the angle of tilt of the surface may be calculated by the instruction CAT for both sets of readings and should be nearly equal. However, subsequent ellipsometer readings will be corrected by the angle of tilt calculated by the last CAT instruction, while for greatest accuracy, the average of the angles computed by the two CAT instructions should be used. This is accomplished by using the instruction CATA to compute the second angle of tilt. The instruction CATA performs the same calculations as CAT, then averages the computed and previously computed values of the angle of tilt. Subsequent ellipsometer readings will then be corrected by the average angle of tilt.

2.5. Film Thickness for a Film of
Known Refractive Index - CD

The instruction CD computes the thickness of a film from values of Δ and ψ . The ellipsometer readings P, A, and Q may also be used as described in the previous section. Before this instruction is used, the following data must have been previously given to the computer or standard values will be used:

1) Wave Length of Light by instruction WL
2) Angle of Incidence by instruction AI
3) Refractive Index of Film by instruction NF
4) Refractive Index of Substrate by instruction NS or CNS
5) Refractive Index of Medium by instruction NM.

If ellipsometer readings are given, the wave plate constants must also be given by instruction WP or CWP, or the standard values will be used.

For example, suppose a film-free surface was measured under water (refractive index of 1.33) with a perfect quarter wave plate set with its fast axis at 45.° from the plane of incidence. Let the values obtained be P = 86.35, A = 25.19 and P = 176.35, A = 154.81 for the two zones. Then let an absorbing film of refractive index 2.5(1-0.3i) be placed on the surface and measurement P = 94.30, A = 24.44 be obtained in one zone. Let the angle of incidence be 65.° and the vacuum wavelength of the light be 5461. Å. Then the following input data will calculate the refractive index of the substrate and the thickness of the film.

	Column No.				
1	10	20	30	40	50
NM	1.33				
NF	2.5			0.3	
AI	65.				
CNS	86.35	25.19	176.35	154.81	45.
CD	94.30	24.44	45.		

Notice that the wavelength is not given since its assigned value is used. The computer output is shown in figure 2.

2.6. Film Thickness and Refractive Index - CND

The instruction CND calculates both the thickness and refractive index of a film from ellipsometer measurements Δ and ψ or from ellipsometer readings P, A, and Q. The data given to the computer before this instruction is the same as for the CD instruction. However, values for the refractive index of the film given by the NF instruction do not have their usual meaning. Consider first the case that the film has a real refractive index (non-absorbing film). Then the CND instruction causes the computer to search for the refractive index of the film between the limits of the initial value and the sum of the initial and increment values.

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Then the search is repeated between the sum of the initial value and increment and the sum of the initial value and twice the increment. This is continued until the final value is reached. For example, if the instruction

NF   1.4   .1   1.6

is followed by a CND instruction, the computer will search for values of n_f between 1.4 and 1.5, and between 1.5 and 1.6. If the increment is not given, the computer will perform a single search between the initial and final values.

The search procedure is explained in section 3.5. The limits of film refractive index given by the NF instruction must be chosen with care. If the limits do not include the solution for the film refractive index, the solution will not be found. On the other hand, if the limits are too broad, a solution may be missed.

An example of instruction CND is given in figure 3. In this example, the values of Δ and ψ are given with the instruction CND. The solution of a film of refractive index of 1.2 and thickness of 1000 Å is found. This solution reduces the error terms ADEL, APSI, and ERROR to be essentially zero. The terms labeled ADSORPTION and WT FRACTION have no meaning since the instruction MIXED was not given (see 2.11). For the meaning of K, see section 4.3.

Consider next the case that the film is absorbing but its value of $\varkappa$ is known. Therefore, only the real part of the refractive index and the thickness of the film are to be determined. In this case the imaginary part of the refractive index of the film is given, starting in column 40 of the NF instruction card and the calculations are the same as the previous case.

In the most difficult case, the film is absorbing and both the real and imaginary part of its refractive index as well as its thickness are to be determined. For this case the range of values of the imaginary part is given by the NF instruction and the real

part of the index and thickness of the film is calculated for each
value. Thus, the instructions

1	10	20	30	40	50	60
NF	1.0		2.0	0.	0.1	1.
CND	152.30	29.00				

will compute the real part of the refractive index and thickness of
the film for assumed values of the imaginary part of the refractive
index of 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8; 0.9, and 1.
The real part of the refractive index is assumed to lie between
1. and 2.. In order to determine which of the calculations corre-
spond to the actual film, additional information is required.
Obviously, three values describing the film cannot be determined
from the two ellipsometer measurement Δ and ψ . For example, if
the thickness of the film was known independently of the ellip-
someter readings, the refractive index of the film can be read
from the calculations. Other possible methods of determining
the refractive index of adsorbing films have been given by
McCrackin and Colson [9].

2.7. Confidence Limits of Film Thickness
and Refractive Index -
CNDE and CNDC

The instruction CNDC performs the same calculations as
instruction CND discussed in the previous section and, in addition,
computes limits of error for the calculated refractive index corre-
sponding to the experimental errors in the ellipsometer measurement
Δ and ψ . The experimental errors, EΔ and Eψ in Δ and ψ must have
been previously given by an EDP instruction or their standard
values of 0.015° are used. This instruction is illustrated in
figure 4.

The 95% confidence limits of the experimental errors based on a large number of degrees of freedom must be used for $E\Delta$ and $E\psi$. That is, the true value of Δ lies in the range $\Delta-E\Delta$ to $\Delta+E\Delta$ with 95% probability, and likewise for ψ. An ellipse is then calculated such that the true values of Δ and ψ will lie within it with 95% probability. Figure 5 shows the ellipse for the conditions of figure 4. (When the errors are equal, this ellipse becomes a circle.)

After calculating the best values for the refractive index n_f and the thickness d_f of the film from the measured Δ and ψ readings, the computer chooses eight evenly-spaced pairs of values from the probability ellipse and computes values of n_f and d_f for each pair. An example is shown in figure 4. The best way to represent these values is to plot n_f versus d_f as shown in figure 6. The points define a curve (approximately an ellipse) surrounding the best value. The true values of n_f and d_f lie within this curve with 95% probability.

This error analysis only takes the errors in the ellipsometer readings into account. Other errors, such as errors in the refractive indexes of the medium and substrate, errors in the angle of incidence, etc., will, of course, increase the error in the calculated values of n_f and d_f.

2.8. Calculations Involving Multiple Films - FILM

The calculations previously described may also be performed for a number of films on the substrate. Three films on a substrate are represented in figure 7. In order to compute the values of Δ and ψ for reflection from this surface, the optical constants and thickness of the three films and the optical constants of the medium and substrate must be given. The films are numbered starting from the surrounding medium. The optical constants of the surrounding medium, film no. 1, and the substrate are given by NM, NF, and NS or CNS instructions as previously described. The thickness of film

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number 1 is treated in the same way as previously described for a single film, i.e., it is given with the CTABLE instruction when the CTABLE instruction is used, or is calculated by the CD, CND, CNDE, or CNDC instructions. The optical constants and thicknesses of the films are given by the FILM instruction. With this instruction: FILM starts in column 1, the number of the film starts in column 10, the thickness of the film in column 20, and the optical constants of the film, n and $\varkappa$, start in columns 30 and 40. Up to 900 films may be specified.

2.9. Inhomogeneous Films - IFILM

All the previously described computations are for homogeneous films, i.e., films for which the optical constants are the same at all points in the film. However, inhomogeneous films for which the optical constants vary along the thickness of the film may be accurately approximated by multiple homogeneous films [9] by use of the instruction FILM described in the previous section. To illustrate, consider a film 100 Å thick whose optical constants vary from n=1, $\varkappa$=0 adjacent to the surrounding medium to n=3, $\varkappa$=1.4 adjacent to the substrate. Let the variation be linear with distance. Then the film may be approximated by 10 homogeneous films as shown in figure 8. Let the optical constants of the substrate be n=3 and $\varkappa$=1.4 and the other parameters of the system have their standard values. Then the reflection coefficients and Δ and ψ for reflection from the film are calculated by the instructions given below.

1	10	20	30	40
NS	3.			1.4
NF	1.1			.07
FILM	2.	10.	1.3	.21
FILM	3.	10.	1.5	.35
FILM	4.	10.	1.7	.49
FILM	5.	10.	1.9	.63
FILM	6.	10.	2.1	.77
FILM	7.	10.	2.3	.91
FILM	8.	10.	2.5	1.05
FILM	9.	10.	2.7	1.19
FILM	10.	10.	2.9	1.33
CTABLE	10.			

The results are shown in figure 9. Approximating this inhomogeneous film with 60 homogeneous films gives $\Delta=117.625°$ and $\psi=30.852°$. Thus, approximating this inhomogeneous film by 10 homogeneous films gave results accurate to $0.1°$ in this case.

The amount of input data for this type of calculation may be reduced by using the instruction IFILM. The data given with IFILM are the number of homogeneous films to be used to represent the inhomogeneous film, the thickness of the inhomogeneous film, the optical constants of the surface and the inhomogeneous film in contact with the immersion medium, and the optical constants of the surface of the film in contact with the substrate. However, film number 1 (the film next to the surrounding medium) is not assigned a thickness or optical constants by IFILM. Thus, the previous calculation may be obtained from the data:

1	10	20	30	40	50	60
NS	3.		1.4			
NF	1.					
IFILM	10.	100.	1.	0.	3.	1.4
CTABLE	0.					

The inhomogeneous film is represented by films 2 to 11. Film number 1 is given zero thickness so has no effect on the results. The values given with IFILM are the number of homogeneous films used to approximate the inhomogeneous film, the thickness of the inhomogeneous film, the values of n and $\varkappa$ at the top (next to surrounding medium) of the inhomogeneous film, and the values of n and $\varkappa$ at the bottom (next to substrate) of the inhomogeneous film, respectively. (See table 2, page 5.) Note that all data, including the number of films, must contain a decimal point.

2.10. Multiple Reflections of the Light

The sensitivity of ellipsometer readings to a thin film on a reflecting surface may be increased by reflecting the light from the surface a number of times. An example of this technique, as well as a discussion of the increase of sensitivity, has been given by Stromberg, Passaglia, and Tutas [10]. To analyze such results the number of reflections may be entered, starting in column 10, on a NREP instruction. The number of reflections must have a decimal point even though it is an integer. All following calculations will then be performed for multiple reflection of the light.

Notice that this instruction is not necessary for the multiple reflections of the light that occur from the surfaces of multiple films, but only for the case that the light emergent from reflection from the surface is again incident on and reflected from the surface.

2.11. Films Composed of a Mixture of Materials

In some applications of ellipsometry, the film being studied is a mixture of a material with the medium above the film. For example, polymer films adsorbed from a solvent on a solid surface [10]

consist of a mixture of the polymer and solvent. As another example, a rough clean substrate may be approximated by the system of the substrate, a film consisting of a mixture of the substrate and the medium, and the medium. For these applications, after the refractive index of the film, n_f , is determined by ellipsometry, the fraction of the film composed of the material and the amount of material per unit area of the surface is desired. These quantities are computed by the instructions CD, CND, CNDC, and CNDE. The amount of the material per unit area of the surface in units of mg/cm^2 is printed in the column labeled ADSORPTION and the weight fraction of material in the film is printed in the column labeled WT FRACTION.

In order for these calculations to be meaningful, the density of the medium, ρ_1 , the density of the material in the film, ρ_p , and the refractive index, n_p , of the material in the film must have been previously given by the instruction MIXED (see table 2 on page 5). The refractive index of the material in the film of the medium are assumed to be real.

The calculations are described in Section 3.

2.12. New Pages, Reset of Variables, and Comments

The instruction PAGE will start a new page of output. For the Fortran V version of the program, comments may be punched in columns 10 to 80 on the same card and will appear on the new page of output. For the Fortran IV version, the comment must be punched on a card following the card containing the instruction PAGE. For this case, any location on the card is satisfactory.

The instruction RESET has the same function as the instruction PAGE and in addition resets all the parameters to the values given in table 3. This instruction placed between two sets of calculations insures that none of the data given for the first set will be used in the second set of calculations.

In addition, for the Fortran V version of the program, any card that does not contain one of the instructions listed in table 2 starting at the first column of the card will be printed as a comment. Therefore, comments may be freely interpreted with the data cards. For the Fortran IV version of the program, comments can only be inserted following a PAGE or RESET instruction.

The instruction STØP is placed at the end of the program.

2.13. Optical Constants of an Adsorbing Film of Given Thickness - CNK, FT

The instruction CNK computes values of n and $\varkappa$ of a film from ellipsometer readings. Values of Δ or ψ or the ellipsometer readings are given with the CNK instruction in the same way as described in section 2.3 for instructions CD, CND, etc. The instruction CNK must be preceded by instructions FT, NF, and NS or CNS. Also, CWP or WP must be given if ellipsometer readings are given with the CNK instruction and NM, AI, and WL instructions if values other than the assumed values are to be used for the refractive index of the medium, the angle of incidence, and the wavelength of the light.

The instruction FT gives the thickness or thicknesses of the film for which the optical constants are to be calculated. The values given with the FT instruction are the same as for the CTABLE instruction (table 2).

The values given with the NF instruction give the ranges in which the computer will search for values of n and $\varkappa$ that correspond to the given ellipsometer measurements. Multiple solutions may be found, in which case, means other than the ellipsometer measurements must be used to chose the correct solution. The incremental values for n and $\varkappa$ given with the NF instruction determine the fineness of the search for the values of n and $\varkappa$. If two solutions for n and $\varkappa$ exist, the n values or $\varkappa$ values must differ by more than the incremental values for both solutions to be found.

An example of these instructions is given in figure 10. The assumed values are used for the index of the medium, angle of incidence, and wavelength of light. For every given value of film thickness, three solutions for n and $\varkappa$ (NF and KAPPA) are found in this example. The accuracy to which they are determined is given in the ΔNF and ΔKAPPA columns.

Thus, for these data, the exact solutions of n and $\varkappa$ may differ by up to .0002 and .00002, respectively, from the solutions given.

For each solution of n and $\varkappa$ and each film thickness, values of Δ and ψ are calculated. The differences between these calculated values and the values given with the CNK instruction are given in the ΔDELTA and ΔPSI columns. These values shall be less than the inaccuracies of the given values of Δ and ψ for the solution to be satisfactory. If Δ and ψ are correct to $0.01°$, some of the solutions, for example the first solution, are not satisfactory. These data could be rerun with smaller incremental values for n and $\varkappa$ on the NF instruction in order to locate the solutions more accurately.

3. Theory and Calculations

The theory of the ellipsometer has been given by various investigators [1-8]. Therefore, only special points of the theory necessary to understand the calculations performed by this program will be given.

3.1. Computation of Δ and ψ From Ellipsometer Readings

Let P, A, and Q be the azimuths of the polarizer, analyzer, and wave plate, respectively, for extinction of the light by the ellipsometer. For the calculations described in this section, the components of the ellipsometer must be arranged in the order of light source, polarizer, wave plate, reflecting surface, analyser,

and light detector. All azimuths are measured counter-clockwise from the plane of incidence looking into the light beam.

The wave plate is characterized by the ratio, T_c, of the transmittance along its fast axis to the transmittance along its slow axis* and the relative phase retardation, Δ_c, along the axes. In the following equation it is characterized by the complex number

$$\rho_c = T_c \exp(-i\Delta_c) = T_c \cos\Delta_c - iT_c \sin\Delta_c \qquad (1)$$

that has been previously computed. The surface is characterized by the complex value

$$\rho = R_p/R_s = \tan\psi \exp(i\Delta) \qquad (2)$$

where R_p and R_s are the complex reflection coefficients for light polarized parallel and normal to the plane of incidence of the light beam. The value of ρ is to be calculated from readings P, A, and Q, and ρ_c. This calculation is based on the formulas derived by Holmes and Feucht [7]. Modifying their equations 19 and 21 for the conventions used in this report for measurement of P, A, and Q gives

$$\rho = \frac{\tan A \left[\tan Q + \rho_c \tan (P-Q)\right]}{\rho_c \tan Q \tan (P-Q) - 1} \qquad (3)$$

for extinction of the light. A derivation of eq (3) is also given in Appendix II.

Δ and ψ are computed from eqs 1 through 3. If two sets of values of P and A are given, ρ is computed for each set and the average of the two values used to compute Δ and ψ.

---

* When the previous program was written, the importance of T_c in ellipsometry was not recognized, thus no correction for it was included in the calculations.

3.2. Computation of Constants T_c and Δ_c of the Wave Plate

For computation of the constants of the wave plate, two sets of readings of P and A (P_1 and A_1 and P_2 and A_2), that produce extinction of light for the same value of Q are required. Then, by eq 3

$$\rho = \frac{\tan A_1 \left[\tan Q + \rho_c \tan (P_1-Q)\right]}{\rho_c \tan Q \tan (P_1-Q) -1}$$

$$= \frac{\tan A_2 \left[\tan Q + \rho_c \tan (P_2-Q)\right]}{\rho_c \tan Q \tan (P_2-Q) -1} \quad .$$

Solving for ρ_c gives

$$\rho_c = \frac{B \pm j \left[-B^2 - \tan (P_1-Q) \tan (P_2-Q)\right]^{\frac{1}{2}}}{- \tan (P_1-Q) \tan (P_2-Q)} \tag{4}$$

where

$$B = \frac{\tan A_1 \left[\tan (P_2-Q) \tan Q - \tan (P_1-Q)/\tan Q\right]}{2 (\tan A_1 - \tan A_2)}$$

$$- \frac{\tan A_2 \left[\tan (P_1-Q) \tan Q - \tan (P_2-Q)/\tan Q\right]}{2 (\tan A_1 - \tan A_2)} \quad . \tag{5}$$

Using eq 1 we find

$$T_c = \frac{1}{\pm\left[-\tan (P_1-Q) \tan (P_2-Q)\right]^{\frac{1}{2}}} \quad . \tag{6}$$

Since T_c is real and positive, $\tan (P_1-Q) \tan (P_2-Q)$ must be negative and the plus square root is used. Also,

$$\tan \Delta_c = \frac{\pm\left[-B^2 - \tan (P_1-Q) \tan (P_2-Q)\right]^{\frac{1}{2}}}{B} \quad . \tag{7}$$

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Δ_c is defined as the phase of light transmitted along the fast axis of the wave plate minus the phase of light transmitted along its slow axis. Therefore, $0 \leq \Delta_c \leq 180°$, so $\sin\Delta_c$ is positive.

Then, by eq 1, the imaginary part of ρ_c is negative. This requires the negative sign for the imaginary term in eq 4 to be used since the denominator has been shown to be positive. Thus,

$$\tan \Delta_c = \frac{+[-B^2 - \tan (P_1-Q) \tan (P_2-Q)]^{\frac{1}{2}}}{B} . \tag{8}$$

3.3. Computation of the Angle of Tilt of the Reflecting Surface

For this calculation, the reflecting surface is assumed to be rotated through a small angle δ around an axis of the intersection of the specimen and the plane of incidence. This rotation or tilting of the specimen has many effects. The angle of incidence to the surface will be changed, but by a negligible amount for small angles of tilt. The direction of the reflected light beam will be changed but is assumed to still pass through the aperatures in the instrument. The main effect will be a reading error of the azimuths of the polarizer, analyzer, and wave plate. Since these elements are alined with respect to the reflecting surface, a tilt of the surface by an angle δ will change the readings of these azimuths by δ . That is

$$
\begin{aligned}
P_1 &= P_1' + \delta & P_2 &= P_2' + \delta \\
A_1 &= A_1' + \delta & A_2 &= A_2' + \delta \\
Q &= Q' + \delta
\end{aligned}
\tag{9}
$$

where P_1', A_1', P_2', A_2', and Q' are readings of the azimuths and P_1, A_1, P_2, A_2, and Q are the true azimuths that would be measured by a properly alined instrument.

By eq 3, for the first set of readings

$$\rho = \frac{\tan\,(A_1{}'+\delta)[\tan\,(Q'+\delta) + \rho_c\,\tan\,(P_1{}'-Q')]}{\rho_c\,\tan\,(Q'+\delta)\,\tan\,(P_1{}'-Q')-1} \cdot \qquad (10)$$

The tangents are expanded in δ and only the term in δ retained, since δ is small.

$$\tan\,(A_1{}'+\delta) \cong \tan A_1{}' + \delta/\cos^2 A'$$

$$\tan\,(Q'+\delta) \cong \tan Q' + \delta/\cos^2 Q' \qquad (11)$$

Eqs 11 are substituted in eq 10 and the result simplified to give

$$\rho = \frac{\alpha_1 + \beta_1\delta}{\gamma_1} \qquad (12)$$

where

$$\alpha_1 = \tan A_1{}'\,[\tan Q' + \rho_c\,\tan\,(P_1{}' - Q')]$$

$$\gamma_1 = \rho_c\,\tan\,(P_1{}' - Q')\,\tan Q'$$

$$\beta_1 = \alpha_1/(\sin A_1{}') +$$

$$[\tan A_1{}'-\alpha_1\rho_c\tan(P_1{}'-Q')\,/\,\gamma_1]\,/\,\cos^2 Q' \, \cdot \qquad (13)$$

Similar formulas apply to the other set (P_2, A_2, and Q) so

$$\rho = \frac{\alpha_1 + \beta_1\delta}{\gamma_1} = \frac{\alpha_2 + \beta_2\delta}{\gamma_2} \cdot \qquad (14)$$

Solving for the angle of tilt gives

$$\delta = \frac{\alpha_2\gamma_1 - \alpha_1\gamma_2}{\beta_1\gamma_2 - \beta_2\gamma_1} \cdot \qquad (15)$$

When δ is calculated, the azimuths are corrected by eq 9 and ρ is calculated by eq 3.

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3.4. Calculation of the Thickness of a Film from Δ and ψ

This calculation has been previously described [4], but since the final formulas were not given, they are summarized here.

The total reflection coefficients R^p and R^s for light polarized parallel and perpendicular to the plane of incidence are given by

$$R^p = \frac{r_{12}^p + r_{23}^p Y}{1 + r_{12}^p r_{23}^p Y}$$

$$R^n = \frac{r_{12}^n + r_{23}^n Y}{1 + r_{12}^n r_{23}^n Y} \qquad (16)$$

where r_{12}^p, r_{23}^p, r_{12}^n, and r_{23}^n are the reflection coefficients between medium and film (indices 1 and 2) and between the film and substrate (indices 2 and 3).

$$Y = \exp[-4\pi i \, n_2 \, \cos\varphi_2 d_2/\lambda] \qquad (17)$$

where n_2 and d_2 are the index of refraction and thickness of the film and φ_2 is the angle for light in the film given by

$$\cos\varphi_2 = [1 - (n_1 \sin\varphi_1/n_2)^2]^{\frac{1}{2}} . \qquad (18)$$

The ellipsometer readings determine

$$\rho = \tan\psi \, \exp(i\Delta) = R^p/R^s . \qquad (19)$$

From eqs 16 and 19,

$$EY^2 + BY + C = 0 , \qquad (20)$$

where

$$E = \rho r_{21}^p \, r_{32}^p \, r_{32}^n - r_n^{21} \, r_{32}^p \, r_{32}^n$$

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$$B = \rho(r^n_{32} + r^p_{21}\, r^n_{21}\, r^p_{32}) - r^{32}_p - r^p_{21}\, r^n_{21}\, r^n_{32}$$

$$C = \rho r^n_{21} - r^p_{21} \;.\qquad\qquad (21)$$

The two solutions of eq 20

$$Y_1 = [-B + (B^2 - 4EC)^{\frac{1}{2}}]\,\big/\,2E \qquad\qquad (22)$$

$$Y_2 = [-B - (B^2 - 4EC)^{\frac{1}{2}}]\,\big/\,2E \qquad\qquad (23)$$

are calculated. Then, from each solution a value for the film thickness d_2 is calculated. These values, called D2C1 and D2C2 are calculated by subroutine CALDX.

These values are complex numbers. Since the film thickness is a real number, the imaginary part is due to error in either the ellipsometer readings or the values of the refractive indices or in the angle of incidence used for the calculation, so must be small. Therefore, the value of D2C1 or D2C2 with the smallest imaginary part is taken as the correct solution. The real part is taken as the film thickness while the imaginary part is taken as a measure of error.

3.5. Calculation of Both the Refractive Index and Thickness of a Film From Values of Δ and ψ

The preceding section described the calculation of the thickness of a film for a given value of the refractive index of a film. Two complex numbers, D2C1 and D2C2, were obtained for the film thickness. The real parts of the numbers were taken as the film thickness and the corresponding imaginary parts as measures of error.

The subroutine SØLN2 determines the refractive index of the film that will minimize the absolute error of the error term.

For simplicity, we consider that the index of the film is real, i.e., $\varkappa=0$. The calculations may also be performed for a given value of $\varkappa$.

The method requires limits, $n_2{}'$ and $n_2{}''$, for the refractive index n_2 of the film, such that $n_2{}' < n_2{}''$. First, the complex film thickness D2Cl is computed with $n_2{}'$ and $n_2{}''$ used for the index. Since the error term, the imaginary part of D2Cl, is zero for the correct value of n_2, it is expected to change sign as n_2 is varied from $n_2{}'$ to $n_2{}''$. Therefore, if the error terms for $n_2{}'$ and $n_2{}''$ have the same sign, it is assumed that no solution for n_2 exists using D2Cl for the film thickness. See figure 11a.

If the error terms have different signs for indices $n_2{}'$ and $n_2{}''$, the error term is evaluated for the intermediate index $n_2{}''' = (n_2{}' + n_2{}'')/2$. Then the interval containing the index n_2 is narrowed by consideration of signs of the error terms. For example, suppose that the signs of the error terms for the indices $n_2{}'$, $n_2{}'''$, $n_2{}''$ are -, -, +, respectively. Then the error term changes sign from $n_2{}'''$ to $n_2{}''$ so the solution for n_2 for which the error term is zero must lie in this range. That is $n_2{}''' < n_2 < n_2{}''$.

The value of $n_2{}'''$ is then tested to determine if it is sufficiently close to the solution for n_2. This is done by computing values of Δ and ψ using the real part of D2Dl for the film thickness. Of course, use of the complex value of D2Cl for the film thickness would give the experimental values of Δ and ψ, but dropping the imaginary part will change the computed values of Δ and ψ. The value of $n_2{}'''$ is then judged to be sufficiently close to the solution for n_2 if the computed values of Δ and ψ are both within 0.005° of the experimental values. If the differences between the computed and experimental values of Δ and ψ are larger than 0.005°, the range is further reduced until they agree to within .005°. (This value of 0.005° can be changed by the ELDP instruction.) The process is then repeated using D2C2.

Note that the values given by the ELDP instruction determine the closeness of the search for the refractive index n_2 of the film. They should be less than the experimental errors of Δ and ψ, but if they are too small, the computation time will be excessive.

Figure 11a shows a possible relationship of the error term to assumed values of the film index. For the limiting values of n_2' and n_2'' of the index, the signs of the error terms are different (- and +) so the computer will search for a solution by computing the error term for the intermediate index n_2'''. The signs of the error terms corresponding to n_2', n_2''', and n_2'' are -, -, and +, respectively. The solution is then correctly determined to lie between n_2''' and n_2'' and this range will be subdivided. The procedure is seen to converge to the solution n_2.

Cases in which the procedure fails are shown in figures 11b to 11d. In figure 11b the error terms are of the same sign (positive) for both n_2' and n_2'' so the computer assumes that no solution exists. However, there is a solution, n_2, outside the assumed range. In this case, too narrow a range for n_2 was used.

In figure 11c the error terms corresponding to the limits n_2' and n_2'' are also of the same sign (positive) so no solution will be found although two solutions between n_2' and n_2'' exist. In this case, the assumed range was too broad. If the range has been subdivided and both sections searched for a solution, both solutions for n_2 would have been obtained.

In figure 11d the error terms for n_2' and n_2'' have different signs so the computer will search for a solution by first computing the error term for index n_2'''. The signs of the error corresponding to n_2', n_2''', and n_2'' are +, -, -, so the computer will continue the search in the interval n_2' to n_2''' and converge to the solution. However, the two solutions between n_2''' and n_2'' will be missed. Again, the range of the index must be subdivided to obtain all the solutions.

3.6. Confidence Limits for the Refractive Index and Thickness of a Film

The preceding section described the calculation of the refractive index and thickness of a film from measured values of Δ and ψ as performed by the instruction CND. Instruction CNDC performs the same calculations and, in addition, calculates the uncertainty in the refractive index and thickness due to uncertainty in the values of Δ and ψ.

Let the measured values of Δ and ψ be Δ_0 and ψ_0 and let their 95 percent confidence limits be $\Delta_0 - \delta\Delta$ to $\Delta_0 + \delta\Delta$ and $\psi_0 - \delta\psi$ to $\psi_0 + \delta\psi$. That is, the true value of Δ lies between $\Delta_0 - \delta\Delta$ and $\Delta_0 + \delta\Delta$ with 95 percent probability, and similarly for ψ. ($\delta\Delta$ and $\delta\psi$ equal 1.96 times the standard deviations of Δ and ψ when based on a large number of degrees of freedom.) Then both Δ and ψ will lie within the joint confidence ellipse (also called contour ellipse) $(\Delta - \Delta_0)^2 / (\delta\Delta)^2 + (\psi - \psi_0)^2 / (\delta\psi)^2 = 1.560$ with 95 percent probability* [11, 12]. An example is shown in figure 5. For each value of Δ and ψ on the ellipse, values of n_2 and d_2, the refractive index and thickness of the film, may be calculated. Plotting these values of n_2 versus d_2, a curve, approximately an ellipse, is obtained as illustrated in figure 6. This curve is the 95 percent joint confidence curve for n_2 and d_2; i.e., the true values of n_2 and d_2 lie within this curve with 95 percent probability.

The instruction CNDC determines eight points of the joint confidence curve for n_2 and d_2. The maximum and minimum values of n_2 and d_2 are also printed as their individual confidence limits. The instruction CNDE performs the same calculations as CNDC but prints only the individual confidence limits of n_2 and d_2.

---

*The equation of the joint confidence ellipse is generally written in terms of standard deviations. For convenience, we have expressed it in terms of 95 percent confidence limits.

The confidence limits for Δ and ψ, $\delta\Delta$ and $\delta\psi$, are given by an EDP instruction before the CNDC or CNDE instruction. If an EDP instruction is not given, the value $0.015°$ is used for both $\delta\Delta$ and $\delta\psi$.

3.7. Volume Fractions and Total Amount of Material for a Film Composed of a Mixture of Two Materials

Consider a film that is a mixture of the immersion medium of refractive index n_1 and density ρ_1 and a material of index n_p and density ρ_p. Let the refractive index of the film that has been calculated be n_f. We desire to compute the weight fraction, f, of the material in the film.

The specific refraction, S_f, of the film is additive in the specific refractions of the medium, S_1, and the material, S_p. Thus

$$S_f/\rho_f = f\, S_p/\rho_p + (1-f)\, S_1/\rho_1 \, , \tag{24}$$

where ρ_f is density of the film and $S_f = (n_f^2-1)/(n_f^2+2)$ and similarly for S_1 and S_p. To determine the density of the film, we have the volume of a unit weight of the film as $f/\rho_p + (1-f)\,\rho_1$ assuming additivity of the partial volumes of the components of the film. Therefore, the density of the film is

$$\rho_f = 1/[f/\rho_p + (1-f)/\rho_1] \, . \tag{25}$$

Substituting in the previous equation and solving for f gives

$$f = \frac{\rho_p}{\rho_p + (S_f-S_p)\rho_1/(S_1-S_f)} \, . \tag{26}$$

The amount of material per unit area of film is $\rho_f d_2 f$ where d_2 is the thickness of the film. If the densities are in g/cm^3 and the film thickness in $\mathring{A}$, the amount of material per unit area of film in mg/cm^2 is given by $10^{-5}\,\rho_f df$.

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3.8. Computation of Ellipsometer
Readings From Δ and ψ

Substituting eqs 1 and 2 in eq 3 and rearranging gives

$$\frac{\tan A}{\tan \psi} = \frac{(\cos\Delta + i\,\sin\Delta)\,[T_c\,\tan Q\,\tan(P-Q)(\cos\Delta_c - i\,\sin\Delta_c)-1]}{\tan Q + T_c\,\tan(P-Q)(\cos\Delta_c - i\,\sin\Delta_c)} . \quad (27)$$

This expression is reduced to the form of a real and imaginary term. Then, the imaginary term must be zero since $\tan A/\tan\psi$ is real. Solving gives

$$\tan(P-Q) = (-R \pm \sqrt{R^2+1}\,)/T_c , \quad (28)$$

where

$$R = \frac{\tan Q\,\sin(\Delta - \Delta_c) - \sin(\Delta + \Delta_c)/\tan Q}{2\,\sin\Delta} \quad (29)$$

or

$$P = \arctan[(-R \pm \sqrt{R^2+1})\,/T_c] + Q . \quad (30)$$

Two values of P are thus calculated. A value of A may be calculated by eq 27 for each value of P.

3.9. Computation of n and $\varkappa$ of a
Film of Given Thickness

This computation is best described by considering the instructions

NS	2.5					
FT	50.					
NF	1.1	0.1	1.3	0.2	0.2	0.2
CNK	90.5	32.				

The computer searches for a value of n between 1.1 and 1.3 and a value of $\varkappa$ between 0.2 and 0.6 for a film of 50 Å thickness that will give values of Δ and ψ near 90.5° and 32°. First, the computer increases the range of n and $\varkappa$ by their increments. That is, the range of n becomes 1.1-0.1 to 1.3+.1 and the range of $\varkappa$ becomes 0.2-0.2 to 0.6+0.2. This is graphically illustrated below.

```
        .8  │  x      x      x      x      x

        .6  │  x      *      *      *      x

 𝜘      .4  │  x      *      0      *      x

        .2  │  x      *      *      *      x

       0.0  │  x      x      x      x      x
            └─────────────────────────────────
              1.0    1.1    1.2    1.3    1.4    ·

                             n
```
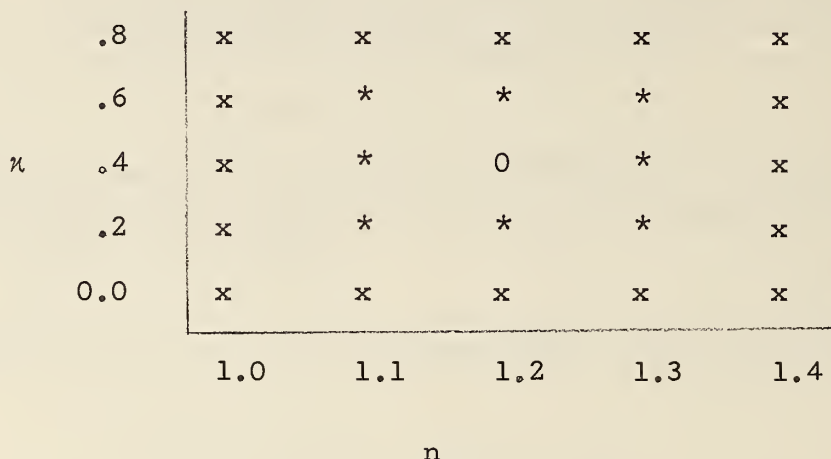
Increasing the ranges of n and $\varkappa$ prevents solutions near the boundary of the range being missed in the searching procedure.

For every pair of values of n and $\varkappa$ in this figure an error term $|\rho_c - \rho_e|$ is computed. In this error term, ρ_c is the value of ρ computed for the value of n, $\varkappa$ and thickness of the film, and ρ_e is the value of ρ corresponding to the values of Δ and ψ (eq 1) given with the CNK instruction. This error term is zero only when the values of n and $\varkappa$ are a solution, and is small when n and $\varkappa$ are near a solution. Therefore, the computation consists of searching for values of n and $\varkappa$ that minimize the error time.

This is accomplished by comparing each error term with the error term at surrounding points. If the error term is less than that at the surrounding points, a minimum is assumed to occur near the value of n and $\varkappa$ for the error term. For example, in the above figure, if the error term for n=1.2 and $\varkappa$=0.4 (represented by 0) is

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less than the surrounding error terms represented by *, a minimum
of the error term is tentatively assumed to occur in the range of
n=1.1 to 1.3 and $\varkappa$=0.2 to 0.6. All interior points of the grid of
n and $\varkappa$ values are thus tested.

The next step is to search the range of n and $\varkappa$ to locate the
minimum. This procedure is illustrated by the following figure.

$\varkappa$	7 x	24 0	8 x	25 0	9 x
	19 0	20 0	21 0	22 0	23 0
	4 x	17 0	5 x	18 0	6 x
	12 0	13 0	14 0	15 0	16 0
	1 x	10 0	2 x	11 0	3 x
		26 0	27 0	28 0	

n

This figure represents the ranges of n and $\varkappa$ for which a mini-
mum is found to occur. That is, the error terms at points 1 to 9,
F_1 to F_9 (represented by x on the figure) have been calculated and
the error term to point 5, F_5, has been found to be less than F_1,
F_2, F_3, F_4, F_6, F_7, F_8, and F_9. The procedure is to calculate the
error term at point 13, F_{13}. If it is greater than F_5, F_{14} is
calculated. If F_{14} is also greater than F_5, F_{15} is calculated,
and so forth. If F_{13}, F_{14}, F_{15}, F_{18}, F_{22}, F_{21}, F_{20}, and F_{17} are
all greater than F_5, they define a new reduced range for the
minimum and the process is repeated.

Consider the case that one of the terms, say F_{15}, is less than F_5. Then F_{15} is also less than F_2, F_3, F_6, and F_{14} since these terms are greater than F_5. Terms F_{11}, F_{16}, and F_{18} are then calculated. If these terms are all greater than F_{15}, a new reduced range centered around F_{15} is found and the process is repeated.

Next, consider the case that one of these terms, say F_{11}, is less than F_{15}. In this case terms F_{26}, F_{27}, and F_{28} are computed. If these terms are all greater than F_{11}, a range centered around F_{11} is found. However, if one of these terms, say F_{26}, is less than F_{11}, another process to follow the minimum is used. All eight terms surrounding F_{26} are calculated and if any of them is less than F_{26}, its eight surrounding terms are calculated and compared with its value. This secondary process is repeated five times. If an error term less than its eight surrounding terms is obtained, the process of reducing the range continues. If not, the process is considered to fail and a diagnostic message printed.

The process of reducing the range is repeated ten times, thereby reducing the original range by a factor of about 2000. These calculations are performed by the subroutine MIN2V and the error terms are calculated by the function FUNC.

Oldham [14] has programed and tested another method for determining the optical properties of adsorbing films of given thickness from ellipsometer readings. His method is a generalization for complex variables of Newton's method of finding roots of a function. His method probably finds solutions with less calculation than the method used in this program. However, it is more likely to fail in finding solutions and does not ordinarily give multiple solutions as does the method used in this program.

4. The Fortran Program

This computer program was originally written in Fortran V for use with the Univac 1108 computer. Because some of the features of this Fortran compiler do not apply to other Fortran compilers, the program in Fortran IV is given in Section 4.1. The data input preceding is identical for both programs except for the instructions discussed in Section 2.12. With the Fortran IV program the first card of the data and the card following the PAGE and RESET instructions must be a comment card, and no other comment cards may be used in the program. Also, comments may not be placed on the PAGE and RESET instruction cards. These restrictions are required because the instruction of the form, READ (0,i) List, in Fortran V is not generally available in Fortran IV.

The Fortran IV program used logical unit 5 for input and logical unit 6 for output. These logical unit numbers may have to be changed for some computers.

For both versions of the program, complex and real values are combined in arithmetic statements with the result being complex.

The Fortran V version of the program and both versions on cards are available from the author.

```
C      CALCULATION FOR ELLIPSOMETER
C        FOR IFILM, THE NUMBER OF FILMS ADD. RESET IS NECESSARY TO ERASE FILMS
C   CHANGED TO USE KAPPA INSTEAD OF IMAGINARY PART OF REFRACTIVE INDEX
       DIMENSION IDT(14),FNSI(2),DFNS(2),FNSE(2),FNSX(2),TN(8),TD(8)
       DIMENSION INST(31)
       COMMON FN1,S1,C1,N,FNX(900),D(900),FN2,CRP,CRN,CRP32,CRN32,WL,
      1 RP21,RN21,DEL,PSI,C2,C3,FN2I(2),DFN2(2),FN2E(2),FN2X(2),T1,T2,T3,
      2 T4,D2,DELDX,PSIDX, ELDEL,ELPSI,DENP,FNP,DEN1,MX,K,IS
       COMPLEX C2,C3,CI,CIP1,CN,CNM1,CRN,CRN21,CRN32,CRP,CRP21,CRP32
       COMPLEX FN2,FNX,FNS, RHO,RN,RN21,      RP,RP21,      RC,SRC
       COMPLEX T1,T2,T3,T4,RHOC,RHO1,RHO2,CAT,ALP1,ALP2,BET1,BET2
       COMPLEX GAM1,GAM2,CAT
C              INSTRUCTIONS TO BE COMPARED WITH INSTRUCTIONS GIVEN WITH
C                           DATA
C         M=      1         2         3         4         5         6
       DATA INST/6HPAGE  ,6HNM   ,6HNF   ,6HNS   ,6HAI   ,6HWL   ,
C        7         8         9        10        11        12        13
      1 6HWP    ,6HNREF  ,6HEDP   ,6HELDP  ,6HRESET ,6HFILM  ,6HMIXED ,
C        14        15        16        17        18        19        20
      2 6HCTABLE,6HCD    ,6HCND   ,6HCNDE  ,6HCNDC  ,6HCNS   ,6HCWP   ,
C        21        22        23        24        25        26        27
      3 6HCDN   ,6HCDNE  ,6HCDNC  ,6HAT    ,6HCAT   ,6HCATA  ,6HIFILM ,
C        28        29       30  31
      4 6HALINE ,6HSTOP  ,2HFT,3HCNK/
C      SRC IS SMALL REFLECTION COEFFICIENT (WITHOUT CONSIDERING
C              UNDERLYING LAYERS)
       SRC(A,B)=(A-B)/(A+B)
C             SIN,COS,ATAN,TAN FOR ANGLES IN DEGREES
       SIND (X)=SIN(X/57.29578)
       COSD (X)=COS(X/57.29578)
       ATAND (X)=ATAN(X)*57.29578
       TAND(X)=SIND(X)/COSD(X)
C      S IS USED FOR CALCULATING SPECIFIC REFRACTION
       S(XN)=(XN*XN-1.)/(XN*XN+2.)
C              GIVE STANDARD VALUES TO VARIABLES
   10 FN1I=1.
      DFN1=0.
      FN1E=0.
      AT=0.
      ALP=0.
      ALA=0.
      ALQ=0.
      FN2I(1)=1.
      FN2I(2)=0.
      DFN2(1)=0.
      DFN2(2)=0.
      FN2E(1)=0.
      FN2E(2)=0.
      FNSI(1)=1.
      FNSI(2)=0.
      DFNS(1)=0.
      DFNS(2)=0.
      FNSE(1)=0.
      FNSE(2)=0.
      AII=70.
      AIE=0.
      WLI=5461.
```

```
              DWL=0.
              WLE=0.
              RHOC=(0.,-1.)
              TC=1.
              DELC=90.
              DEN1=1.
              DENP=1.
              FNP=1.5
              N=2
              ELDEL=.002
              ELPSI=.002
              D2I=0.
              DD2=0.
              D2F=0.
              FN=1.
              EDEL=.015
              EPSI=.015
C                 READ AND PRINT TITLE CARD
   12 READ(5,15) IDT
   15 FORMAT(13A6,A2)
      WRITE(6,17) IDT
   17 FORMAT(1H1,14A6)
C                 READ AND PRINT CARD OF DATA
   20 READ(5,25) L,Z1,Z2,Z3,Z4,Z5,Z6
   25 FORMAT(A6,3X,6F10.0)
      WRITE(6,27) L,Z1,Z2,Z3,Z4,Z5,Z6
   27 FORMAT(1H ,A6,3X,6F15.5)
C                 COMPARE L WITH INSTRUCTIONS TO FIND M.
      DO 30 M=1,31
   30    IF(L.EQ.INST(M))  GO TO 35
      GO TO 20
C        M=   1   2   3   4   5   6   7   8   9  10 11  12  13  14  15  16
   35 GO TO(12,50,70,80,90,100,110,120,130,140,10,150,160,305,170,170,
C       17  18  19  20  21  22  23  24  25  26  27  28  29  30  31
     1 170,170,170,730,170,170,170,250,750,750,270,260,810,305,170),M
C           INSTRUCTION NM,REFRACTIVE INDEX OF MEDIUM
   50 FN1I=Z1
      DFN1=Z2
      FN1E=1.000001*Z3
      GO TO 20
C       INSTRUCTION NF, REFRACTIVE INDEX OF TOP FILM
   70 FN2I(1)=Z1
      DFN2(1)=Z2
      FN2E(1)=1.000001*Z3
      FN2I(2)=Z4
      DFN2(2)=Z5
      FN2E(2)=1.000001*Z6
C         IF DFN2(1) IS LEFT BLANK ON DATA CARD, SUBSTITUTE A VALUE OF
C             DFN2(1) SO THAT ONLY ONE CALCULATION WILL BE PREFORMED.
      IF(ABS(DFN2(1)).EQ.0.) DFN2(1)=1.000002*ABS(FN2E(1)-FN2I(1))
C         INSTRUCTION NS, REFRACTIVE INDEX OF SUBSTRATE
   80 FNSI(1)=Z1
      DFNS(1)=Z2
      FNSE(1)=1.000001*Z3
      FNSI(2)=Z4
      DFNS(2)=Z5
      FNSE(2)=1.000001*Z6
      GO TO 20
C         INSTRUCTION AI, ANGLE OF INCIDENCE
   90 AII=Z1
      DAI=Z2
      AIE=1.000001*Z3
```

```
          GO TO 20
C         INSTRUCTION WL,   WAVE LENGTH OF LIGHT
  100 WLI=Z1
      DWL=Z2
      WLE=1.000001*Z3
      GO TO 20
C         INSTRUCTION WP, CONSTANTS OF WAVE PLATE
  110 TC=Z1
      DELC=Z2
      RHOC=TC*CEXP((0.,-1.)*DELC/57.29578)
      GO TO 20
C         INSTRUCTION NREF, NUMBER OF REFLECTIONS OF THE LIGHT
  120 FN=Z1
      GO TO 20
C         INSTRUCTION EDP, CONFIDENCE FIMITS FOR DELTA AND PSI
  130 EDEL=Z1
      EPSI=Z2
      GO TO 20
C         INSTRUCTION ELDP, ERROR LIMITS FOR DELTA AND PSI
  140 ELDEL=Z1
      ELPSI=Z2
      GO TO 20
C     INSTRUCTION FILM ,NUMBER, THICKNESS AND REFRACTIVE INDEX OF FILM
  150 I=1.000001*Z1+1
      D(I)=Z2
      FNX(I)=CMPLX(Z3,-Z3*ABS(Z4))
      N=MAX0(N,I)
      GO TO 20
C         INSTRUCTION MIXED, DATA FOR MIXED FILMS
  160 DEN1=Z1
      DENP=Z2
      FNP=Z3
      GO TO 20
C     VALUES OF DELTA AND PSI OR OF P,A,AND Q HAVE BEEN GIVEN
C         USE PREVIOUS VALUES OF DEL AND PSI IF NO DATA IS GIVEN,Z1=Z2=0
C             IF FIRST VALUE(Z1) =0,USE PREVIOUSLY GIVEN VALUES OF
C                         DELTA AND PSI
  170 IF(ABS(Z1).EQ.0.) GO TO 310
      IF(ABS(Z5).EQ.0.) GO TO 180
C             Z5 NOT =0, SO P1,A1,P2,A2,Q ARE GIVEN
C             COMPUTE TWO VALUES OF RHO
      Z1=Z1+AT+ALP
      Z2=Z2+AT+ALA
      Z3=Z3+AT+ALP
      Z4=Z4+AT+ALA
      Z5=Z5+AT+ALQ
      WRITE(6,27) L,Z1,Z2,Z3,Z4,Z5
  174 RHO1=TAND(Z2)*(TAND(Z5)+TAND(Z1-Z5)*RHOC)/(TAND(Z1-Z5)*TAND(Z5)*
     1     RHOC-1.)
      RHO2=TAND(Z4)*(TAND(Z5)+TAND(Z3-Z5)*RHOC)/(TAND(Z3-Z5)*TAND(Z5)*
     1     RHOC-1.)
C             AVERAGE VALUES OF RHO,COMPUTE VALUES OF DELTA AND PSI
      RHO=(RHO1+RHO2)/2.
      DEL1=ATAN2(AIMAG(RHO1),REAL(RHO1))*57.29578
      PSI1=ATAND(CABS(RHO1))
      DEL2=ATAN2(AIMAG(RHO2),REAL(RHO2))*57.29578
      PSI2=ATAND(CABS(RHO2))
      WRITE(6,175) DEL1,PSI1,DEL2,PSI2
  175 FORMAT(6H DEL1=,F12.6,6H PSI1=,F12.6,6H DEL2=,F12.6,
     1 6H PSI2=,F12.6)
      IF(FN.EQ.1.) GO TO 210
      GO TO 200
```

```
C               IF Z3=0, DELTA AND PSI ARE GIVEN,OTHERWISE P,A,Q ARE GIVEN
  180 IF(ABS(Z3).EQ.0.) GO TO 190
      Z1=Z1+AT+ALP
      Z2=Z2+AT+ALA
      Z3=Z3+AT+ALQ
      WRITE(6,27) L,Z1,Z2,Z3
  185 RHO=TAND(Z2)*(TAND(Z3)+TAND(Z1-Z3)*RHOC)/(TAND(Z1-Z3)*TAND(Z3)*
     1      RHOC-1.)
      IF(FN.EQ.1.) GO TO 210
      GO TO 200
  190 DEL=Z1
      PSI=Z2
      RHO=TAND(PSI)*CEXP((0.,1.)*DEL/57.29578)
      IF(FN.EQ.1.) GO TO 310
C               CORRECT FOR NUMBER OF REFLECTIONS IF FN NOT =1
  200 RHO=CEXP(1./FN*CLOG(RHO))
  210 DEL=ATAN2(AIMAG(RHO),REAL(RHO))*57.29578
      PSI=ATAND(CABS(RHO))
      IF(M.EQ.25 .OR. M.EQ.26)  GO TO 755
  215 WRITE(6,220) DEL,PSI
  220 FORMAT(6H   DEL=,F13.6,5H PSI=,F13.6)
      GO TO 310
C          INSTRUCTION AT, ANGLE OF TILT OF SAMPLE
  250 AT=Z1
      GO TO 20
C        INSTRUCTION ALINE, ALINEMENT CORRECTIONS
  260 ALP=Z1
      ALA=Z2
      ALQ=Z3
      GO TO 20
C         INSTRUCTION IFILM, CALCULATES THICKNESSES AND REFRACTIVE
C          INDICES OF A SERIES OF FILMS
  270 XNF=Z1
      TH=Z2
C       REMOVE ALL PREVIOULSY DESIGNATED FILMS.
C    WITHOUT NEXT CARD, FILMS WILL BE PLACED BETWEEN PREVIOUSLY
C         DESIGNATED FILMS AND SUBSTRATE
      N=2
C        DN AND DK ARE INCREMENTS OF REFRACTIVE INDEX AND K
      DN=(Z5-Z3)/XNF
      DK=(Z6-Z4)/XNF
C          COMPUTE INDEX AND K (KAPPA) OF TOP FILM
      Z3=Z3+DN/2.
      Z4=Z4+DK/2.
C        INDEX OF TOP FILM IS N1, INDEX OF BOTTOM FILM IS N
      N1=N+1
      NF=1.000001*XNF
      N=N+NF
      DO 280 I=N1,N
      D(I)=TH/NF
      FNX(I)=CMPLX(Z3,-Z3*Z4)
      Z3=Z3+DN
  280 Z4=Z4+DK
      GO TO 20
C    THICKNESS OF TOP FILM AND ,OPTIONALLLY, SETTING OF WAVE PLATE
  305 D2I=Z1
      DD2=Z2
      D2E=1.000001*Z3
      Q=Z4
      IF(M.EQ.30) GO TO 20
C     SET INITIAL  VALUES
  310 FN1=FN1I
```

```
    311 AI=AII
    312 S1=SIND(AI)
        C1=COSD(AI)
        IF(M.EQ.19) GO TO 710
    315  WL=WLI
        WRITE (6,316) FN1,AI,WL,TC,DELC
    316 FORMAT(17H0INDEX OF MEDIUM=,F10.5,21H  ANGLE OF INCIDENCE=,F10.3,
       1 14H  WAVE LENGTH=,F10.2,5H  TC=,F10.5,7H  DELC=,F10.3)
        IF(M.EQ.14) GO TO 320
        IF(M.EQ.31) GO TO 318
C            PRINT TABLE HEADINGS EXCEPT FOR CTABLE OR CNK
        WRITE(6,317)
    317 FORMAT(123H0    THICK  NF REAL      KAPPA  ADSORPTION     D DEL      D P
       1SI      ERROR      NF-NM      NS-NF WT FRACTION  NS REAL    KAPPA
       2 K)
        GO TO 320
C        PRINT HEADINGS FOR INSTRUCTION CNK
    318 PRINT 319
    319 FORMAT(1H0,8X,2HNF,15X,5HKAPPA,9X,4HD NF,11X,7HD KAPPA,9X,
       1  5HERROR,3X,7HD DELTA,5X,5HD PSI,10X,5HTHICK)
    320  NP1=N+1
C                SET VALUES FOR REFRACTIVE INDEX OF SUBSTRATE
    325  FNSX(1)=FNSI(1)
    326  FNSX(2)=FNSI(2)
    327  FNX(NP1)=CMPLX(FNSX(1),-FNSX(2)*FNSX(1))
C            COMPUTE  REFLECTION COEF  BETWEEN LAYERS 3 AND 4
        IF(N.EQ.2) GO TO 335
        X=SIND(AI)*FN1
        CN=CSQRT(1.-(X/FNX(N+1))**2)
        CNM1=CSQRT(1.-(X/FNX(N))**2)
        CRP=SRC(FNX(N+1)*CNM1,FNX(N)*CN)
        CRN=SRC(FNX(N)*CNM1,FNX(N+1)*CN)
        IF(N.EQ.3) GO TO 335
        NX=N-3
        I=N-1
        DO 330 J=1,NX
          CIP1=CSQRT(1.-(X/FNX(I+1))**2)
          CI=  CSQRT(1.-(X/FNX(I))  **2)
          RP=SRC(FNX(I+1)*CI,FNX(I)*CIP1)
          RN=SRC(FNX(I)*CI,FNX(I+1)*CIP1)
          T1=FNX(I+1)*CIP1*D(I+1)/WL
          CRP=RC(RP,CRP,T1)
          CRN=RC(RN,CRN,T1)
    330 I=I-1
    335 IF(M.EQ.31) GO TO 850
    340 FN2X(2)=FN2I(2)
    342 FN2X(1)=FN2I(1)
    343 FN2=CMPLX(FN2X(1),-FN2X(2)*FN2X(1))
C        CALCULATE REFLECTION COEF BETWEEN LAYERS 2 AND 3
        CALL  CRC
        IF(M.EQ.14) GO TO 350
        K=1
C                EXCEPT FOR CTABLE,CALCULATE VALUES,T1 AND T2, OF FILM
C                            THICKNESS
        CALL  CALDX (T1,T2)
        IF(M.EQ.15) GO TO 455
C                EXCEPT FOR CTABLE OR CD,CALCULATE COMPLEX VALUES,T3 AND
C                    T4 OF FILM THICKNESS FOR UPPER VALUE OF FILM
C                        REFRACTIVE INDEX
        FN2=CMPLX(FN2X(1)+DFN2(1),-FN2X(2)*(FN2X(1)+DFN2(1)))
        CALL  CRC
        CALL  CALDX(T3,T4)
```

```
C   IS=1 FOR NO SOLUTION FOUND   IS=2 FOR SOLUTION FOUND
      IS=1
      IF(( AIMAG(T1).GT.0..AND.AIMAG(T3).LT.0.).OR.(AIMAG(T1).LT.0..AND.
     1  AIMAG(T3).GT.0.)) GO TO   485
C         NO SOLUTION FOR N2 FOR FIRST SOLUTION OF QUADRATIC
  345 IF((AIMAG(T2).GT.0..AND.AIMAG(T4).LT.0.).OR.(AIMAG(T2).LT.0.AND.
     1  AIMAG(T4).GT.0.))   GO TO 487
C         NO SOLUTION FOR N2 FOR SECOND SOLUTION OF QUADRATIC
  347 IF(IS.EQ.2) GO TO 670
C   NO SOLUTION FOUND, TRY OTHER QUADRANTS FOR SQRT IN CALDX
      K=3
      FN2=CMPLX(FN2X(1),-FN2X(2)*FN2X(1))
      CALL   CRC
      CALL   CALDX (T1,T2)
      FN2=CMPLX(FN2X(1)+DFN2(1),-FN2X(2)*(FN2X(1)+DFN2(1)))
      CALL   CRC
      CALL   CALDX(T3,T4)
      IF(( AIMAG(T1).GT.0..AND.AIMAG(T3).LT.0.).OR.(AIMAG(T1).LT.0..AND.
     1  AIMAG(T3).GT.0.)) GO TO   490
  348 IF((AIMAG(T2).GT.0..AND.AIMAG(T4).LT.0.).OR.(AIMAG(T2).LT.0.AND.
     1  AIMAG(T4).GT.0.))   GO TO 489
      GO TO 670
C         TABLES OF DEL AND PSI FOR CTABLE
  350 WRITE(6,360)
  360 FORMAT(1H0,3X,5HTHICK,4X,3HDEL,5X,3HPSI,4X,14HRF.CF.PARALLEL,6X,
     1         12HRF.CF.NORMAL,4X,2HNF,4X,5HKAPPA,2X,2HNS,5X,5HKAPPA,4H,
     2         2HP1,5X,2HA1,5X,2HP2,5X,2HA2)
  390 D2=D2I
  400 CRP21=RC(RP21,CRP32,FN2*C2*D2/WL)
      CRN21=RC(RN21,CRN32,FN2*C2*D2/WL)
      RHO=CRP21/CRN21
      IF(FN.NE.1.) RHO=CEXP(1./FN*CLOG(RHO))
      DEL=ATAN2(AIMAG(RHO),REAL(RHO))*57.29578
      IF(REAL(RHO).LT.0. .AND. ABS(AIMAG(RHO)).LT. 1.0E-6) DEL=180.
      PSI=ATAND(CABS(RHO))
      XM1=CABS(CRP21)
      THETA1=ATAN2(AIMAG(CRP21),REAL(CRP21))*57.29578
      IF(REAL(CRP21).LT.0. .AND. ABS(AIMAG(CRP21)).LT.1.0E-6)THETA1=180.
      XM2=CABS(CRN21)
      THETA2=ATAN2(AIMAG(CRN21),REAL(CRN21))*57.29578
      IF(REAL(CRN21).LT.0. .AND. ABS(AIMAG(CRN21)).LT.1.0E-6)THETA2=180.
      FN2R=REAL(FN2)
      FNXR=REAL(FNX(N+1))
      FK2=-AIMAG(FN2)/REAL(FN2)
      FKX=-AIMAG(FNX(N+1))/REAL(FNX(N+1))
      IF(ABS(Q).NE.0.) GO TO 420
      WRITE(6,410) D2,DEL,PSI,XM1,THETA1,XM2,THETA2,FN2R,FK2,FNXR,FKX
  410 FORMAT(1H F8.1,2F8.3,2(F9.5,F9.3),4F7.4,4F7.2)
      GO TO 450
C         Q NOT 0, COMPUTE P AND A READINGS FOR VALUE OF Q
C     CORRECT Q FOR TILT AND ALINEMENT
  420 TQ=TAND(Q+AT+ALQ)
      IF(ABS(DEL).LT.1.0E-6) GO TO 430
      R=(TQ*SIND(DEL-DELC)-SIND(DEL+DELC)/TQ)/2./SIND(DEL)
      TP1=(-R+SQRT(R*R+1))/TC
      TP2=(-R-SQRT(R*R+1))/TC
      P1=ATAND(TP1)+Q-ALP+ALQ
      P2=ATAND(TP2)+Q-ALP+ALQ
      A1=ATAND(REAL(RHO*(TP1*TQ*RHOC-1.)/(TQ+TP1*RHOC)))-AT-ALA
      A2=ATAND(REAL(RHO*(TP2*TQ*RHOC-1.)/(TQ+TP2*RHOC)))-AT-ALA
      GO TO 440
C     USE LIMITING FORMS OF EQUATIONS FOR DEL NEARLY =0.
```

```
    430 P1=Q-ALP+ALQ
        P2=Q-ALP+ALQ-90.
        A1=ATAND(REAL(RHO/TQ))-AT-ALA
        A2=ATAND(REAL(RHO*TQ))-AT-ALA
C           REDUCE ANGLES TO LIE BETWEEN 0 AND 180 DEGREES
    440 P1=AMOD(P1+360.,180.)
        A1=AMOD(A1+360.,180.)
        P2=AMOD(P2+360.,180.)
        A2=AMOD(A2+360.,180.)
        WRITE(6,410) D2,DEL,PSI,XM1,THETA1,XM2,THETA2,FN2R,FK2,FNXR,
       1 FKX,P1,A1,P2,A2
    450 D2=D2+DD2
        IF(D2.LT.D2E) GO TO 400
        GO TO  670
C       COMPUTE FILM THICKNESS  M=15        CD
C       PICK THICKNESS WITH  SMALLEST IMAGINARY PART
    455 IF(ABS(AIMAG(T2)).LT.ABS(AIMAG(T1)))   GO TO 460
        D2=REAL(T1)
        ERROR=AIMAG(T1)
        K=1
        GO TO 470
    460 D2=REAL(T2)
        ERROR=AIMAG(T2)
        K=2
C       COMPUTE DEL AND PSI FOR CALCULATED FILM THICKNESS D2
    470 CRP21=RC(RP21,CRP32,FN2*C2*D2/WL)
        CRN21=RC(RN21,CRN32,FN2*C2*D2/WL)
        RHO1=CRP21/CRN21
        PSIX=ATAND(CABS(RHO1))-PSI
        DELX=57.29578*ATAN2(AIMAG(RHO1),REAL(RHO1))-DEL
        DIFN21=REAL(FN2)-FN1
        DIFN32=REAL(FNX(N+1))-REAL(FN2)
C       WEIGHT FRACTION AND WEIGHT OF MATERIAL IN UNIT AREA OF FILM
        FRACTN=DENP/(DENP+(S(REAL(FN2))-S(FNP))*DEN1/(S(FN1)-S(REAL(FN2))))
       1 )
        WTMT=1.0E-5*D2*FRACTN/(FRACTN/DENP+(1.-FRACTN)/DEN1)
        FN2R=REAL(FN2)
        FNXR=REAL(FNX(N+1))
        FK2=-AIMAG(FN2)/REAL(FN2)
        FKX=-AIMAG(FNX(N+1))/REAL(FNX(N+1))
        WRITE(6,480) D2,FN2R,FK2,WTMT,DELX,PSIX,ERROR,DIFN21,DIFN32,
       1 FRACTN,FNXR,FKX,K
    480 FORMAT(1H ,F8.1,2F9.5,1PE12.4,0P2F9.3,F12.5,3F10.5,2F9.5,I6)
        GO TO   670
C         CALCULATE SOLUTION FOR N2 FOR FIRST SOLUTION OF QUADRATIC
    485 K=1
        GO TO 490
    487 K=2
        GO TO 490
    489 K=4
C               MX=16 SO THAT SOLN2 WILL PRINT
    490 MX=16
        CALL SOLN2
        MX=M
        IF(M.EQ.16 .OR. M.EQ.21 .OR. IS.EQ.1) GO TO (345,347,348,670),K
C         PRINT BLANK SPACE
        WRITE(6,27)
C         CALCULATE ERROR LIMITS FOR N2 AND D2
        DEL0=DEL
        PSI0=PSI
        DEL=DEL0+1.249*EDEL
        CALL SOLN2
```

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```
          TN(1)=REAL(FN2)
          TD(1)=D2
          DEL=DEL0-1.249*EDEL
          CALL SOLN2
          TN(2)=REAL(FN2)
          TD(2)=D2
          DEL=DEL0
          PSI=PSI0+1.249*EPSI
          CALL SOLN2
          TN(3)=REAL(FN2)
          TD(3)=D2
          PSI=PSI0-1.249*EPSI
          CALL SOLN2
          TN(4)=REAL(FN2)
          TD(4)=D2
          DEL=DEL0+0.883*EDEL
          PSI=PSI0+0.883*EPSI
          CALL SOLN2
          TN(5)=REAL(FN2)
          TD(5)=D2
          DEL=DEL0-0.883*EDEL
          CALL SOLN2
          TN(6)=REAL(FN2)
          TD(6)=D2
          DEL=DEL0+0.883*EDEL
          PSI=PSI0-0.883*EPSI
          CALL SOLN2
          TN(7)=REAL(FN2)
          TD(7)=D2
          DEL=DEL0-0.883*EDEL
          CALL SOLN2
          TN(8)=REAL(FN2)
          TD(8)=D2
          FN2MIN=AMIN1(TN(1),TN(2),TN(3),TN(4),TN(5),TN(6),TN(7),TN(8))
          FN2MAX=AMAX1(TN(1),TN(2),TN(3),TN(4),TN(5),TN(6),TN(7),TN(8))
          D2MIN=AMIN1(TD(1),TD(2),TD(3),TD(4),TD(5),TD(6),TD(7),TD(8))
          D2MAX=AMAX1(TD(1),TD(2),TD(3),TD(4),TD(5),TD(6),TD(7),TD(8))
          WRITE(6,495) D2MIN,D2MAX,FN2MIN,FN2MAX
      495 FORMAT(39H0CONFIDENCE LIMITS OF FILM THICKNESS ISF8.1,3H TOF8.1/
         1        69H CONFIDENCE LIMITS OF THE REAL PART OF INDEX OF REFRACTI
         2ON OF FILM ISF12.5,3H TO F12.5)
          GO TO (345,347,348,670),K
      670 FN2X(1)=FN2X(1)+DFN2(1)
          IF(FN2X(1).LT.FN2E(1))  GO TO 343
      700 FN2X(2)=FN2X(2)+DFN2(2)
          IF(FN2X(2).LT.FN2E(2))  GO TO 342
          FNSX(2)=FNSX(2)+DFNS (2)
          IF (FNSX(2).LT.FNSE(2))  GO TO 327
          FNSX(1)=FNSX(1)+DFNS(1)
          IF(FNSX(1).LT.FNSE(1))  GO TO 326
          WL=WL+DWL
          IF(WL.LT.WLE)           GO TO 320
      705 AI=AI+DAI
          IF(AI.LT.AIE)           GO TO 312
          FN1=FN1+DFN1
          IF(FN1.LT.FN1E)         GO TO 311
          GO TO 20
C         CALCULATE REFRACTIVE INDEX OF SUBSTRATE CNS
      710 FNS=FN1*S1/C1*CSQRT(1.-4.*RHO*S1**2/(RHO+1.)**2)
          FNSI(1)=REAL(FNS)
          FNSI(2)=-AIMAG(FNS)/FNSI(1)
          FNSE(1)=0.
```

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            FNSE(2)=0.
            WRITE(6,720) FNSI,DEL,PSI
        720 FORMAT(20H0INDEX OF SUBSTRATE=F9.4,F9.4,2H  ,2X,4HDEL=,
           1 F9.3,2X,4HPSI=F9.3)
            IF(FNSI(2).LT.0.) GO TO 725
            GO TO 705
        725 WRITE(6,727)
        727 FORMAT(62H0KAPPA IS SET EQUAL TO 0,SINCE A NEGATIVE VALUE WAS CALC
           1ULATED)
            FNSI(2)=0.
            GO TO 705
C           COMPUTE CONSTANTS OF WAVE PLATE          CWP
C       ASSUMES ANGLE OF TILT AT IS ZERO
        730 Z1=Z1+ALP
            Z2=Z2+ALA
            Z3=Z3+ALP
            Z4=Z4+ALA
            Z5=Z5+ALQ
            WRITE(6,27) L,Z1,Z2,Z3,Z4,Z5
            IF(ABS(Z3-Z5).LT.0.1 .OR. ABS(Z1-Z5).LT.0.1) GO TO 745
        735 B=(TAND(Z2)*(TAND(Z3-Z5)*TAND(Z5)-TAND(Z1-Z5)/TAND(Z5))-TAND(Z4)*
           1 (TAND(Z1-Z5)*TAND(Z5)-TAND(Z3-Z5)/TAND(Z5)))/2./
           2 (TAND(Z2)-TAND(Z4))
            DELC= ATAN2(SQRT(-B*B-TAND(Z1-Z5)*TAND(Z3-Z5)),B)*57.29578
            TC=1./SQRT(-TAND(Z1-Z5)*TAND(Z3-Z5))
            RHOC=TC*CEXP((0.,-1.)*DELC/57.29578)
            RHO =TAND(Z2)*(TAND(Z5)+TAND(Z1-Z5)*RHOC)/(TAND(Z1-Z5)*TAND(Z5)*
           1     RHOC-1.)
            DEL=57.29578*ATAN2(AIMAG(RHO),REAL(RHO))
            PSI=ATAND(CABS(RHO))
            WRITE(6,740) TC,DELC,DEL,PSI
        740 FORMAT(4H TC=,F10.5,9H DELTA C=,F10.5,7H DELTA=,F15.5,5H PSI=,
           1      F15.5)
            GO TO 20
        745 WRITE (6,747)
        747 FORMAT( 73H0CONSTANTS OF WAVE PLATE CAN NOT BE ACCURATELY CALCULAT
           1ED FROM ABOVE DATA)
            GO TO 20
C             CALCULATE ANGLE OF TILT OF STAGE ON ELLIPSOMETER CAT IS COMP
C             ANGLE WITH REAL PART ANGLE AND IMAGINARY PART ERROR
        750 Z1=Z1+ALP
            Z2=Z2+ALA
            Z3=Z3+ALP
            Z4=Z4+ALA
            Z5=Z5+ALQ
            WRITE(6,27 ) L,Z1,Z2,Z3,Z4,Z5
            TP1=TAND(Z1-Z5)
            TA1=TAND(Z2)
             TP2=TAND(Z3-Z5)
            TA2=TAND(Z4)
            TQ =TAND(Z5)
            ALP1=TA1*(TQ+TP1*RHOC)
            ALP2=TA2*(TQ+TP2*RHOC)
            GAM1=TP1*TQ*RHOC-1.
            GAM2=TP2*TQ*RHOC-1.
            BET1=ALP1/SIND(Z2)/COSD(Z2)+(TA1-ALP1*TP1*RHOC/GAM1)/COSD(Z5)**2
            BET2=ALP2/SIND(Z4)/COSD(Z4)+(TA2-ALP2*TP2*RHOC/GAM2)/COSD(Z5)**2
            CAT=(ALP2*GAM1-ALP1*GAM2)/(BET1*GAM2-BET2*GAM1)*57.29578
            ATX=REAL(CAT)
            Z1=Z1+ATX
            Z2=Z2+ATX
            Z3=Z3+ATX
```

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        Z4=Z4+ATX
        Z5=Z5+ATX
C           COMPUTE RHO,DEL,PSI
        GO TO 174
    755 PRINT 760,CAT,DEL,PSI
    760 FORMAT(15H ANGLE OF TILT=,F13.5,15H DEGREES,ERROR=,F13.5,
       1        7H DELTA=,F15.5,5H PSI=,F15.5)
        IF(M.EQ.26) ATX=(ATX+AT)/2.
        AT=ATX
        GO TO 20
    810 STOP
C   INSTRUCTION CNK  M=31  COMPUTES N AND KAPPA OF FILM
    850 D2=D2I
    852 PRINT 855,D2
    855 FORMAT(1H0,90X,F15.1)
    860 CALL MIN2V(FN2I(1),DFN2(1),FN2E(1),FN2I(2),DFN2(2),FN2E(2))
        D2=D2+DD2
        IF(D2.LT.D2E) GO TO 852
        GO TO 20
        END

        SUBROUTINE  SOLN2
C         SOLVES FOR REAL PART OF REFRACTIVE INDEX AND THICKNESS OF
C         A FILM FOR MEASUREMENTS OF DELTA AND PSI
C         ER2 IS ERROR OF SOLUTION,THICK IS FILM THICKNESS,INDEX IN FN2
C         IF K=1 OR 3, FIRST(POSITIVE SIGN) SOLUTION IS USED
C         IF K=2 OR 4, SECOND(NEGATIVE SIGN) SOLUTION IS USED
        COMMON FN1,S1,C1,N,FNX(900),D(900),FN2,CRP,CRN,CRP32,CRN32,WL,
       1 RP21,RN21,DEL,PSI,C2,C3,FN2I(2),DFN2(2),FN2E(2),FN2X(2),T1,T2,T3,
       2 T4,D2,DELX ,PSIX , ELDEL,ELPSI,DENP,FNP,DEN1,M,K,IS
        COMPLEX FNX,FN2,CRP,CRN,CRP32,CRN32,RP21,RN21,C2,C3,T1,T2,T3,T4,
       1 T5,T6,RHO,RC
C         S IS USED FOR CALCULATING SPECIFIC REFRACTION
        S(XN)=(XN*XN-1.)/(XN*XN+2.)
        ATAND(X)=ATAN(X)*57.29578
        X1=FN2X(1)
        X3=FN2X(1)+DFN2(1)
        GO TO (10,20,10,20),K
     10 ER1=AIMAG(T1)
        ER3=AIMAG(T3)
        GO TO 30
     20 ER1=AIMAG(T2)
        ER3=AIMAG(T4)
     30 DO 80 I=1,20
        X2=(X1+X3)/2.
        FN2=CMPLX(X2,-FN2X(2)*X2)
        CALL CRC
        CALL CALDX(T5,T6)
        GO TO (40,50,40,50),K
     40   D2=REAL(T5)
        ER2=AIMAG(T5)
        GO TO 60
     50   D2=REAL(T6)
        ER2=AIMAG(T6)
C          COMPUTE DEL AND PSI FOR FILM THICKNESS D2
     60   RHO=RC(RP21,CRP32,FN2*C2*D2/WL)/RC(RN21,CRN32,FN2*C2*D2/WL)
        DELX =ATAN2(AIMAG(RHO),REAL(RHO))*57.29578-DEL
        PSIX=ATAND(CABS(RHO))-PSI
        IF(ABS(DELX ).LT.ELDEL.AND. ABS(PSIX ).LT.ELPSI)  GO TO 100
C        HAS NOT CONVERGED TO ELDEL AND ELPSI.  CHANGE LIMITS X1,X3
C            IF ER1 AND ER2 HAVE SAME SIGN,X1=X2 AND ER1=ER2,OTHERWISE
C            ER2 AND ER3 HAVE SAME SIGN,X3=X2 AND ER3=ER2
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          IF((ER1.GT.0.0 .AND. ER2.GT.0.0).OR.(ER1.LT.0.0 .AND.
     1    ER2.LT.0.0)) GO TO 70
          X3=X2
          ER3=ER2
          GO TO 80
   70     X1=X2
          ER1=ER2
   80 CONTINUE
   90 D2=1.0E30
      FN2=1.0E30
      RETURN
C     IF FILM THICKNESS D2 IS NEGATIVE,TREAT AS NO SOLUTION
  100 IF(D2.LT.0.) GO TO 90
C         PRINT SOLUTION AND ERROR LIMITS
      IF(M.EQ.17 .OR. M.EQ.22)  GO TO 120
      DIFN21=X2-FN1
      DIFN32=REAL(FNX(N+1))-X2
      FRACTN=DENP/(DENP+(S(X2)-S(FNP))*DEN1/(S(FN1)-S(X2)))
      WTMT=1.0E-5*D2*FRACTN/(FRACTN/DENP+(1.-FRACTN)/DEN1)
      FN2R=REAL(FN2)
      FNXR=REAL(FNX(N+1))
      FK2=-AIMAG(FN2)/REAL(FN2)
      FKX=-AIMAG(FNX(N+1))/REAL(FNX(N+1))
      PRINT 110,D2,FN2R,FK2,WTMT,DELX,PSIX,ER2,DIFN21,DIFN32,
     1 FRACTN,FNXR,FKX,K
  110 FORMAT(1H ,F8.1,2F9.5,1PE12.4,0P2F9.3,F12.5,3F10.5,2F9.5,I6)
      IS=2
  120 RETURN
      END


      SUBROUTINE  CRC
C         CALCULATES CRP32 AND CRN32    REFLECTION COEF OF MEDIUM 2 AND 3
      COMMON FN1,S1,C1,N,FNX(900),D(900),FN2,CRP,CRN,CRP32,CRN32,WL,
     1 RP21,RN21,DEL,PSI,C2,C3,FN2I(2),DFN2(2),FN2E(2),FN2X(2),T1,T2,T3,
     2 T4,D2,DELDX,PSIDX, ERDEL,ERPSI,DENP,FNP,DEN1
      COMPLEX FNX,FN2,CRP,CRN,CRP32,CRN32,RP21,RN21,C2,C3,T1,T2,T3,T4
      COMPLEX RC,RP32,RN32
      SRC(A,B)=(A-B)/(A+B)
      X=FN1*S1
      C2=CSQRT(1.-(X/FN2)**2)
      C3=CSQRT(1.-(X/FNX(3))**2)
      RP21=SRC(FN2*C1,FN1*C2)
      RN21=SRC(FN1*C1,FN2*C2)
      IF(N.EQ.2) GO TO 10
      RP32=SRC(FNX(3)*C2,FN2*C3)
      RN32=SRC(FN2*C2,FNX(3)*C3)
      CRP32=RC(RP32,CRP,FNX(3)*C3*D(3)/WL)
      CRN32=RC(RN32,CRN,FNX(3)*C3*D(3)/WL)
      RETURN
   10 CRP32=SRC(FNX(3)*C2,FN2*C3)
      CRN32=SRC(FN2*C2,FNX(3)*C3)
      RETURN
      END


      COMPLEX FUNCTION RC(R21,CR32,Q  )
C         RC=REFLECTION COEFFICIENT INCLUDING EFFECT OF UNDERLYING LAYERS
C  FOLLOWING CARD IS REQUIRED FOR FORTRAN V ONLY
      COMPLEX CEXP,CLOG,CSQRT
      COMPLEX R21,CR32,Q  ,T
      T=CEXP((0.,-12.56637)*Q)
C         Q=N2*COS(PHI2)*D/WL          (0.,-12.56637)=-4*PI*J
      RC=(R21+CR32*T)/(1.+R21*CR32*T)
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      RETURN
      END


      SUBROUTINE  CALDX(D2C1,D2C2)
C  FOLLOWING CARD IS REQUIRED FOR FORTRAN V ONLY
      COMPLEX CEXP,CLOG,CSQRT
C     CALCULATES FILM THICKNESS AND ERROR TERMS
      COMMON FN1,S1,C1,N,FNX(900),D(900),FN2,CRP,CRN,CRP32,CRN32,WL,
     1 RP21,RN21,DEL,PSI,C2,C3,FN2I(2),DFN2(2),FN2E(2),FN2X(2),T1,T2,T3,
     2 T4,D2,DELDX,PSIDX, ERDEL,ERPSI,DENP,FNP,DEN1,M,K
      COMPLEX FNX,FN2,CRP,CRN,CRP32,CRN32,RP21,RN21,C2,C3,T1,T2,T3,T4
      COMPLEX E,B,C,Y1,Y2,D2C1,D2C2,RHO,T5,T6
      RHO=SIN(PSI/57.29578)/COS(PSI/57.29578)*CEXP((0.,1.)*DEL/57.29578)
C       Y=EXP(-2 J DEL2)    LET  E*Y**2+BY+C=0  Y1,Y2 ARE TWO SOLUTIONS
      E=RHO*RP21*CRP32*CRN32-RN21*CRP32*CRN32
      B=RHO*(CRN32+RP21*RN21*CRP32)-CRP32-RP21*RN21*CRN32
      C=RHO*RN21-RP21
      T5=CSQRT(B**2-4.*E*C)
      GO TO (20,20,10,10),K
C    MAKE IMAGINARY PART OF SQUARE ROOT POSITIVE
   10 IF(AIMAG(T5).LT.0.) T5=-T5
   20 Y1=(-B+T5)/2./E
      Y2=(-B-T5)/2./E
      T5=CLOG(Y1)
      T6=CLOG(Y2)
      D2C1=WL*T5/(0.,-12.56637)/FN2/C2
      D2C2=WL*T6/(0.,-12.56637)/FN2/C2
      RETURN
      END


      SUBROUTINE MIN2V(XI,DX,XF,YI,DY,YF)
C       USES FUNCTION FUNC(X,Y) WHICH MUST BE INCLUDED. DETERMINES AND PRINTS
C     VALUES OF X BETWEEN XI AND XF AND VALUES OF Y BETWEEN YI AND YF THAT
C     MINIMIZE FUNC. WILL FIND MULTIPLE MINIMUMS IF THEY ARE SEPARATED
C       BY MORE THAN DX AND DY
      DIMENSION F(50,50)
      COMMON FN1,S1,C1,N,FNX(900),D(900),FN2,CRP,CRN,CRP32,CRN32,WL,
     1 RP21,RN21,DEL,PSI,C2,C3,FN2I(2),DFN2(2),FN2E(2),FN2X(2),T1,T2,T3,
     2 T4,D2,DELDX,PSIDX, ERDEL,ERPSI,DENP,FNP,DEN1,MX,K,IS,RHO
      COMPLEX FNX,FN2,CRP,CRN,CRP32,CRN32,RP21,RN21,C2,C3,T1,T2,T3,T4
      COMPLEX RC,RHO
C     COMPUTE NUMBER OF VALUES OF X AND Y FOR RANGES XI-DX TO XF+DX
C     AND YI-DY TO YF+DY.
      NX=(1.000001*XF-XI)/DX+3
      NY=(1.000001*YF-YI)/DY+3
      IF(NX.GT.50) PRINT 10,DX
   10 FORMAT('0INCREMENT OF X,'E12.5,' IS TOO SMALL')
      IF(NY.GT.50) PRINT 20,DY
   20 FORMAT('0INCREMENT OF Y,'E12.5,' IS TOO SMALL')
C      COMPUTE INITIAL VALUE OF X
      X=XI-DX
C      COMPUTE TABLE F OF FUNCTION FUNC
      DO 40 I=1,NX
         Y=YI-DY
         DO 30 J=1,NY
            F(I,J)=FUNC(X,Y)
C*********DIAGNOSTIC PRINTING***************************************,
C            PRINT 35,I,J,F(I,J)
   30       Y=Y+DY
   35       FORMAT(2I5,E20.7)
   40    X=X+DX
      NX1=NX-1
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          NY1=NY-1
          DO 910 I=2,NX1
          DO 900 J=2,NY1
C     SEARCH FOR MINIMUMS OF F(VALUES LESS THAN ALL  8 SURROUNDING VALUES)
          IF(F(I,J).LT.F(I-1,J-1).AND. F(I,J).LT.F(I-1,J) .AND.
     1    F(I,J).LT.F(I-1,J+1) .AND. F(I,J).LT.F(I,J-1) .AND.
     2    F(I,J).LT.F(I,J+1) .AND. F(I,J).LT.F(I+1,J-1)
     3    .AND. F(I,J).LT.F(I+1,J) .AND.
     4    F(I,J).LT.F(I+1,J+1))GO TO 50
          GO TO 900
   50     XMIN=XI+(I-2)*DX
          YMIN=YI+(J-2)*DY
          FMIN=F(I,J)
C     A MINIMUM FMIN OCCURS NEAR POINT I,J AT XMIN-DX TO XMIN+DX AND
C        YMIN-DY TO YMIN+DY,
C        SUBDIVIDE RANGE TO LOCATE MINIMUM.
          XD=DX/2
          YD=DY/2
C        SUBDIVIDE RANGE 10 TIMES
          DO 550 K=1,10
              F13=FUNC(XMIN-XD,YMIN-YD)
              F14=FUNC(XMIN,YMIN-YD)
              IF(F13.LT.FMIN) GO TO 110
              IF(F14.LT.FMIN) GO TO 120
C        F14 GT FMIN
  105         F15=FUNC(XMIN+XD,YMIN-YD)
              IF(F15.LT.FMIN) GO TO 130
C        F15 GT FMIN
  107         F18=FUNC(XMIN+XD,YMIN)
              IF(F18.LT.FMIN) GO TO 140
              F22=FUNC(XMIN+XD,YMIN+YD)
              IF(F22.LT.FMIN) GO TO 150
C         F22 GT FMIN
              F21=FUNC(XMIN,YMIN+YD)
              IF(F21.LT.FMIN) GO TO 160
C        F21 GT FMIN
              F20=FUNC(XMIN-XD,YMIN+YD)
              IF(F20.LT.FMIN) GO TO 170
              F17=FUNC(XMIN-XD,YMIN)
              IF(F17.LT.FMIN) GO TO 180
C     FMIN LT SURROUNDINGS
              GO TO 500
  110         IF(F14.LT.F13) GO TO 120
C     F13 LT F14 AND FMIN
              F17=FUNC(XMIN-XD,YMIN)
C     IF F17 LT F13, CONTINUE SCAN WITH F15
              IF(F17.LT.F13) GO TO 105
C        F13 LT F14,FMIN,F17
              F12=FUNC(XMIN-2*XD,YMIN-YD)
              IF(F12.LT.F13) GO TO 190
              F10=FUNC(XMIN-XD,YMIN-2*YD)
              IF(F10.LT.F13) GO TO 200
C        F13 IS NEW MINIMUM
              FMIN=F13
              XMIN=XMIN-XD
              YMIN=YMIN-YD
              GO TO 500
C        F14 LT FMIN,F13
  120         F15=FUNC(XMIN+XD,YMIN-YD)
              IF(F15.LT.F14) GO TO 130
              F11=FUNC(XMIN+XD,YMIN-2*YD)
              IF(F11.LT.F14)  GO TO 210
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              F10=FUNC(XMIN-XD,YMIN-2*YD)
              IF(F10.LT.F14)  GO TO 200
              F17=FUNC(XMIN-XD,YMIN)
              IF(F17.LT.F14) GO TO 107
              F18=FUNC(XMIN+XD,YMIN)
              IF(F18.LT.F14) GO TO 140
C         F14 IS NEW MINIMUM
              FMIN=F14
              YMIN=YMIN-YD
              GO TO 500
C       F15 LT FMIN ,F14
   130        F11=FUNC(XMIN+XD,YMIN-2*YD)
              IF(F11.LT.F15) GO TO 210
              F18=FUNC(XMIN+XD,YMIN)
              IF(F18.LT.F15) GO TO 140
              F16=FUNC(XMIN+2*XD,YMIN-YD)
              IF(F16.LT.F15) GO TO 220
C         F15 IS NEW MINIMUM
              FMIN=F15
              XMIN=XMIN+XD
              YMIN=YMIN-YD
              GO TO 500
C        F18 LT FMIN,F15,F14
   140        F16=FUNC(XMIN+2*XD,YMIN-YD)
              IF(F16.LT.F18) GO TO 220
              F22=FUNC(XMIN+XD,YMIN+YD)
              IF(F22.LT.F18) GO TO 150
              F21=FUNC(XMIN,YMIN+YD)
              IF(F21.LT.F18) GO TO 160
              F23=FUNC(XMIN+2*XD,YMIN+YD)
              IF(F23.LT.F18) GO TO 230
C        F18 IS NEW MINIMUM
              FMIN=F18
              XMIN=XMIN+XD
              GO TO 500
C       F22 LT FMIN,F18
   150        F21=FUNC(XMIN,YMIN+YD)
              IF(F21.LT.F22) GO TO 160
              F23=FUNC(XMIN+2*XD,YMIN+YD)
              IF(F23.LT.F22) GO TO 230
              F25=FUNC(XMIN+XD,YMIN+2*XD)
              IF(F25.LT.F22) GO TO 240
C       F22 IS NEW MINIMUM
              FMIN=F22
              XMIN=XMIN+XD
              YMIN=YMIN+YD
              GO TO 500
C       F21 LT FMIN,F22,F18
   160        F25=FUNC(XMIN+XD,YMIN+2*XD)
              IF(F25.LT.F21) GO TO 240
              F20=FUNC(XMIN-XD,YMIN+YD)
              IF(F20.LT.F21) GO TO 170
              F17=FUNC(XMIN-XD,YMIN)
              IF(F17.LT.F21) GO TO 180
              F24=FUNC(XMIN-XD,YMIN+2*YD)
              IF(F24.LT.F21) GO TO 250
C         F21 IS NEW MINUMUM
              FMIN=F21
              YMIN=YMIN+YD
              GO TO 500
C     F20 LT FMIN,F21
   170        F17=FUNC(XMIN-XD,YMIN)
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            IF(F17.LT.F20) GO TO 180
            F24=FUNC(XMIN-XD,YMIN+2*YD)
            IF(F24.LT.F20) GO TO 250
            F19=FUNC(XMIN-2*XD,YMIN+YD)
            IF(F19.LT.F20) GO TO 260
C        F20 IS NEW MINUMUM
            FMIN=F20
            XMIN=XMIN-XD
            YMIN=YMIN+YD
            GO TO 500
C         F17 LT FMIN F20,F21,F13,F14
   180      F12=FUNC(XMIN-2*XD,YMIN-YD)
            IF(F12.LT.F17) GO TO 190
            F19=FUNC(XMIN-2*XD,YMIN+YD)
            IF(F19.LT.F17) GO TO 260
C         F17 IS NEW MINUMUM
            FMIN=F17
            XMIN=XMIN-XD
            GO TO 500
C         F12 LT F13,FMIN,F17
   190      F10=FUNC(XMIN-XD,YMIN-2*YD)
            IF(F10.LT.F12) GO TO 200
            FMIN=F12
            XMIN=XMIN-2*XD
            YMIN=YMIN-YD
   192      FX=FUNC(XMIN-XD,YMIN-YD)
            IF(FMIN.GT.FX) GO TO 194
            FX=FUNC(XMIN-XD,YMIN)
            IF(FMIN.GT.FX) GO TO 196
            FX=FUNC(XMIN-XD,YMIN+YD)
            IF(FMIN.GT.FX) GO TO 198
            GO TO 500
   194      YMIN=YMIN-YD
   196      XMIN=XMIN-XD
            FMIN=FX
            GO TO 300
   198      YMIN=YMIN+YD
            GO TO 196
C      F10 LT F13,F14,F12,FMIN
   200      FMIN=F10
C      CHECK TO SEE THAT F10 IS NEW MINIMUM
            XMIN=XMIN-XD
            YMIN=YMIN-2*YD
   202      FX=FUNC(XMIN-XD,YMIN-YD)
            IF(FMIN.GT.FX) GO TO 204
            FX=FUNC(XMIN,YMIN-YD)
            IF(FMIN.GT.FX) GO TO 206
            FX=FUNC(XMIN+XD,YMIN-YD)
            IF(FMIN.GT.FX) GO TO 208
            GO TO 500
   204      XMIN=XMIN-XD
   206      YMIN=YMIN-YD
            FMIN=FX
            GO TO 300
   208      XMIN=XMIN+XD
            GO TO 206
C      F11 LT F14,F15
   210      F18=FUNC(XMIN+XD,YMIN)
            IF(F18.LT.F11) GO TO 140
            F16=FUNC(XMIN+2*XD,YMIN-YD)
            IF(F16.LT.F11) GO TO 220
            FMIN=F11
```

```
                XMIN=XMIN+XD
                YMIN=YMIN-2*YD
                GO TO 202
C        F16 LT F15,F11,F18
  220           FMIN=F16
                XMIN=XMIN+2*XD
                YMIN=YMIN-YD
  222           FX=FUNC(XMIN+XD,YMIN-YD)
                IF(FMIN.GT.FX) GO TO 224
                FX=FUNC(XMIN+XD,YMIN)
                IF(FMIN.GT.FX) GO TO 226
                FX=FUNC(XMIN+XD,YMIN+YD)
                IF(FMIN.GT.FX) GO TO 228
                GO TO 500
  224           YMIN=YMIN-YD
  226           XMIN=XMIN+XD
                FMIN=FX
                GO TO 300
  228           YMIN=YMIN+YD
                GO TO 226
C         F23 LT F18,F22,FMIN
  230           F25=FUNC(XMIN+XD,YMIN+2*XD)
                IF(F25.LT.F23) GO TO  240
                FMIN=F23
                XMIN=XMIN+2*XD
                YMIN=YMIN+YD
                GO TO 222
C     F25 LT F21,F22,F23,FMIN
  240           FMIN=F25
                XMIN=XMIN+XD
                YMIN=YMIN+2*YD
  242           FX=FUNC(XMIN-XD,YMIN+YD)
                IF(FMIN.GT.FX) GO TO 244
                FX=FUNC(XMIN,YMIN+YD)
                IF(FMIN.GT.FX) GO TO 226
                FX=FUNC(XMIN+XD,YMIN+YD)
                IF(FMIN.GT.FX) GO TO 248
                GO TO 500
  244           XMIN=XMIN-XD
  246           YMIN=YMIN+YD
                FMIN=FX
                GO TO 300
  248           XMIN=XMIN+XD
                GO TO 246
C        F24 LT F21,F20,F17,FMIN
  250           F19=FUNC(XMIN-2*XD,YMIN+YD)
                IF(F19.LT.F24) GO TO 260
                FMIN=F24
                XMIN=XMIN-XD
                YMIN=YMIN+2*YD
                GO TO 242
C        F19 LT F20,F17,FMIN
  260           F17=FUNC(XMIN-XD,YMIN)
                IF(F17.LT.F19) GO TO 180
                FMIN=F19
                XMIN=XMIN-2*XD
                YMIN=YMIN+YD
                GO TO 192
C                     FOLLOW MINIMUM FOR 5 STEPS
  300           DO 400 KK=1,5
                    FX=FUNC(XMIN-XD,YMIN-YD)
                    IF(FX.LT.FMIN) GO TO 310
```

```
                  FX=FUNC(XMIN-XD,YMIN)
                  IF(FX.LT.FMIN) GO TO 320
                  FX=FUNC(XMIN-XD,YMIN+YD)
                  IF(FX.LT.FMIN) GO TO 330
                  FX=FUNC(XMIN,YMIN-YD)
                  IF(FX.LT.FMIN) GO TO 340
                  FX=FUNC(XMIN,YMIN+YD)
                  IF(FX.LT.FMIN) GO TO 350
                  FX=FUNC(XMIN+XD,YMIN-YD)
                  IF(FX.LT.FMIN) GO TO 360
                  FX=FUNC(XMIN+XD,YMIN)
                  IF(FX.LT.FMIN) GO TO 370
                  FX=FUNC(XMIN+XD,YMIN+XD)
                  IF(FX.LT.FMIN) GO TO 380
                  GO TO 500
      310         YMIN=YMIN-YD
      320         XMIN=XMIN-XD
                  GO TO 400
      330         YMIN=YMIN+YD
                  GO TO 320
      340         YMIN=YMIN-YD
                  GO TO 400
      350         YMIN=YMIN+YD
                  GO TO 400
      360         YMIN=YMIN-YD
      370         XMIN=XMIN+XD
                  GO TO 400
      380         YMIN=YMIN+YD
                  GO TO 370
      400         FMIN=FX
C                      A MINIMUM IS NOT FOUND IN 5 STEPS
              GO TO 600
      500         XD=XD/2
                  YD=YD/2
      550         CONTINUE
C                      NEW MINIMUM IS FOUND
              GO TO 700
      560     FORMAT(5E15.6,3I5/(7F15.6))
      600     PRINT 610,K,FMIN,XMIN,YMIN,XD,YD
      610     FORMAT('0 ITERATION NUMBER'I3,' FAILED FOR MINIMUM'E12.5,' AT X
     1=,E12.5,' Y=,E12.5,' RANGES =' 2E12.5)
C****************PRINT VALUES AT MINIMUM
      700     FN2=CMPLX(XMIN,-XMIN*YMIN)
                  T1=RC(RP21,CRP32,FN2*C2*D2/WL)/RC(RN21,CRN32,FN2*C2*D2/WL)
                  DDEL=ATAN2(AIMAG(T1),REAL(T1))*57.29578-DEL
                  DPSI=ATAN(ABS(T1))*57.29578-PSI
          XD=2*XD
          YD=2*YD
              PRINT 800, XMIN,YMIN,XD,YD,FMIN,DDEL,DPSI
      800     FORMAT(' '5F15.5,2F10.3)
      900     CONTINUE
      910     CONTINUE
          RETURN
          END

          FUNCTION FUNC(FRN,FK)
C         COMPUTES VALUES OF DELTA AND PSI, DELC AND PSIC, FOR A FILM
C             OF N=FRN,KAPPA=FK, AND THICKNESS=D2 AND ERROR TERM,FUNC
          COMMON FN1,S1,C1,N,FNX(900),D(900),FN2,CRP,CRN,CRP32,CRN32,WL,
     1 RP21,RN21,DEL,PSI,C2,C3,FN2I(2),DFN2(2),FN2E(2),FN2X(2),T1,T2,T3,
     2 T4,D2,DELDX,PSIDX, ERDEL,ERPSI,DENP,FNP,DEN1,MX,K,IS,RHO
          COMPLEX FNX,FN2,CRP,CRN,CRP32,CRN32,RP21,RN21,C2,C3,T1,T2,T3,T4
```

```
   COMPLEX RC,RHO
      FN2=CMPLX(FRN,-FRN*FK)
      CALL CRC
   FUNC=ABS(RC(RP21,CRP32,FN2*C2*D2/WL)/RC(RN21,CRN32,FN2*C2*D2/WL)
  1   -RHO)
   RETURN
   END
```

4.2. Subprograms

Subprogram	Type	
ABS	Real	Absolute value
AIMAG	Real	Imaginary part of complex argument
AMAX1	Real	Maximum of real arguments
AMIN1	Real	Minimum of real arguments
AMØD	Real	Remainder obtained by dividing first by second argument.
ATAN	Real	Arctangent
ATAN2	Real	Divides first by second argument and calculates arctangent of quotient in proper quadrant.
ATAND	Real	Arctangent given in degrees, statement function
CALDX		Subroutine furnished with program. Calculates two complex values (D2C1 and D2C2) for the thickness of the top film for DEL and PSI given in common. Requires CRN, CRP, CRN32, CRP32, RN21, and RP21, to have been previously calculated. The value of K determines which solution corresponds to D2C1 and D2C2.
CABS	Real	Absolute value of complex argument
CEXP	Complex	Complex exponential
CLØG	Complex	Complex natural logarithm
CMPLX	Complex	Calculates a complex number. The real part of the complex number is the first argument and imaginary part is the second argument.
CØS	Real	Cosine
CØSD	Real	Cosine of angle in degrees, statement function.
CRC	Real	Subroutine furnished with program. Computes C2, C3, RP21, RN21, CRN32, and CRP32.
CSQRT	Complex	Complex square root

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MAXO	Integer	Result is the maximum of the integer arguments.
RC	Complex	Complex function furnished with program. Computes the reflection coefficient from a surface covered by one or many films. Requires the Fresnel reflection coefficient (R21) from the top film, the reflection coefficient (CR32) from the medium under the top film, i.e., either the Fresnel reflection coefficient of the substrate or the reflection coefficient from the second film considering underlying films, and $Q = n_f \cos\varphi_f d_f / \lambda$ where n_f, φ_f, and d_f are the refractive index, angle of reflection, and thickness of film.
REAL	Real	The real part of a complex number.
S	Real	Statement function
SIN	Real	Sine
SIND	Real	Statement function. The sine of an angle given in degrees.
SOLN2		Subroutine furnished by program. Solves by a search procedure for both the real part of the refractive index and thickness of the top film on a surface that will give values of DELX and PSIX (Δ and ψ) that will agree with given values DEL and PSI within tolerance ELDEL and ELPSI. The solution will be printed unless MX=17 or 22. The real part of the refractive index of the film is assumed to lie between FN2X(1) and FN2X(1)+DFN2(1) and the value of kappa of the film is FN2X(2). The solution to be used for the thickness of the film is determined by the value of $\varkappa$. The complex thicknesses of the film and the limits of the range of refractive index to be searches, i.e., at FN2X(1) and FN2X(1)+DFN2(1) must have been calculated and stored in T1, T2, T3, and T4.

If a solution is printed, IS is made equal to 2.

The search procedure is described in Section 3.5. |
SQRT	Real	Square root
SRC	Complex	Statement function used in computing Fresnel reflection coefficients.
TAND	Real	Statement function. The tangent of an angle given in degrees.

4.3. Variables Used in Program

a. Variables in Common

Fortran	Type		
C1	Real	$\cos\varphi_1$	Cosine of angle of incidence
C2	Complex	$\cos\varphi_2$	Cosine of angle of refraction in top film
C3	Complex	$\cos\varphi_3$	Cosine of angle of refraction in 2nd medium
CRN	Complex	R^n	Total reflection coefficient for light polarized normal to the plane of incidence.
CRP	Complex	R^p	Total reflection coefficient for light polarized parallel to the plane of incidence.
CRN32	Complex	R^n_{32}	Total reflection coefficient between mediums 2 and 3.
CRP32	Complex	R^p_{32}	Total reflection coefficient between mediums 2 and 3.
D(900)	Real	d_1	Thicknesses of films
D2	Real	d_2	Thickness of top film
DEL	Real	Δ	Relative phase retardation
DENI	Real	ρ_1	Density of medium 1
DENP	Real	ρ_p	Density of medium p
DFN2(2)	Real	δn_2	Increments for film refractive index
ELDEL	Real		Error limits for Δ
ELPSI	Real		Error limits for ψ
FN1	Real	n_1	Refractive index of medium
FN2	Complex	$\hat{n}_f$ or $\hat{n}_2$	Refractive index of top film
FN2E(2)	Real		Final values to be used for refractive index of top film.
FN2I(2)	Real		Initial values to be used for refractive index of top film.

FN2X(2)	Real		Refractive index of top film. The complex refractive index (FN2) is computed from FN2X.
FNX(900)	Complex	n_1	Refractive index of films other than top film and of the substrate.
FNP	Real	n_p	Refractive index of material in film.
IS	Integer		IS determines if a solution for refractive index of the film has been found by SØLN2. It is originally equal to 1, and is changed to 2 when a solution is found.
K	Integer		In calculating the thickness of a film, two solutions are obtained (see Section 3.4). K identifies the solution used, being 1 for the positive solution given by eq. 22 and 2 for the negative solution given by eq. 23. The square root of (B^2-4EC) is taken so that the real part of the square root is positive. In searching for the refractive index of the film in subroutine SØLN2, if no solution is found for either K=1 or 2 (using either eq. 22 or 23), the square root of (B^2-4EC) is taken so the imaginary part is positive. In some cases, a solution will then be found for the refractive index of the film which is labeled K=3 or 4 corresponding to eq. 22 or 23, respectively.
MX	Integer		Used in SØLN2 to control printing. The solution is printed unless MX=17 or 22. Generally, MX is equal to M.
N	Integer		The number of films on the surface plus 1. Initially, N=2 corresponding to one film.
PSI	Real	ψ	tan ψ is relative reflection coefficient.
PSIX	Complex	$\delta\psi$	Error in ψ
RP21	Complex	r^p_{21}	Fresnel reflection coefficient between medium and film next to medium for light polarized parallel to the plane of incidence.

Fortran	Type	
RN21	Real	r_{21}^n Fresnel reflection coefficient between medium and film next to medium for light polarized normal to the plane of incidence.
S1	Real	$\sin\varphi_1$ Sine of angle of incidence
T1, T2, T3, T4	Complex	Temporary storage
WL	Real	λ Vacuum wavelength of light

b. Complex Variables Not in Common

Fortran		
ALP1		α_1 See Section 3.3
ALP2		α_2 See Section 3.3
BET1		β_1 See Section 3.3
BET2		β_2 See Section 3.3
C2		$\cos\varphi_2$ Cosine of angle of refraction in top film
C3		$\cos\varphi_3$ Cosine of angle of refraction in film or substrate adjacent to top film.
CAT		Complex angle of tilt. See Section 3.3.
CI		$\cos\varphi_i$ Cosine of angle of refraction in medium i.
CIP1		$\cos\varphi_{i+1}$ Cosine of angle of refraction in medium i+1.
CN		$\cos\varphi_n$ Cosine of angle of refraction in the substrate.
CNM1		$\cos\varphi_{n-1}$ Cosine of angle of refraction in the film adjacent to the substrate.
CRN		R^n Reflection coefficient for normal polarization considering underlying films.

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CRN21	R_{21}^n	Reflection coefficient from top film for normal polarization considering underlying films.
CRN32	R_{32}^n	Reflection coefficient from second film or substrate for normal polarization considering underlying layers.
CRP	R^p	Reflection coefficient for parallel polarization considering underlying films.
CRP21	R_{21}^p	Reflection coefficient from top film for parallel polarization considering underlying layers.
CRP32	R_{32}^p	Reflection coefficient from second film or substrate for parallel polarization considering underlying layers.
FNS	n_s	Refractive index of substrate.
GAM1	γ_1	See Section 3.3.
GAN2	γ_2	See Section 3.3.
RHØ	$\rho = R_{21}^p / R_{21}^n$	Ratio of reflection coefficient.
RHØ1	ρ	Calculated from first set of values of P and A.
RHØ2	ρ	Calculated from second set of values of P and A.
RHØC	ρ_c	Complex constant of wave plate defined by eq. 1.
RN	r_n	Fresnel reflection coefficient for light polarized normal to the plane of incidence.
RP	r_p	Fresnel reflection coefficient for light polarized parallel to the plane of incidence.

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Appendix I

Use of the ALINE Instruction in Relation to
Alinement of the Ellipsometer

Carl Fenstermaker

This appendix describes a modification of the alinement proce-
dure of McCrackin, et al [4]. In the procedure described below the
components are not adjusted in their holders to correct errors in
the readings of their associated scales. Instead, errors in the
scale readings are measured and used to correct future readings.
Physical adjustment to 0.01 degree of the components within their
scales is frequently very difficult, requiring tedious small
changes and rechecks to approach the accuracy of readability. This
modified procedure is much faster and the alinement can be done to
the accuracy of the scales on the first trial. Although all future
readings must be corrected, this correction is easily made with the
ALINE instruction.

We define P, A, and Q as the actual azimuthal position of the
plane of transmission of the prisms of polarizer and analyzer and
plane of the fast axis of the wave plate respectively, and P_s, A_s,
and Q_s as the corresponding scale readings. All azimuthal angles
are measured positive counter-clockwise from the plane of incidence
when looking into the light beam.

The corrections used on the ALINE card (ΔP, ΔA, and ΔQ) are
the values which, when added to the scale readings, give the actual
positions of the plane of transmission of the polarizer and
analyzer and the position of the fast axis of the wave plate, so

$$P = P_s + \Delta P \tag{31}$$

$$A = A_s + \Delta A \tag{32}$$

$$Q = Q_s + \Delta Q . \tag{33}$$

As in Section 2.3 "Alinement Procedure" of reference [4], the wave plate is removed, the arms of the ellipsometer set in the straight through position, the scale reading of the polarizer, P_s, set to zero and the azimuth of the analyzer is adjusted to a value near 90° that gives a minimum in the transmitted light. At the minimum the polarizer and analyzer are crossed so that

$$A = P + 90°,$$

or by eqs 31 and 32

$$A_s + \Delta A = \Delta P + 90°$$

since $P_s = 0$.

Defining $\epsilon = A_s - 90°$ gives

$$\Delta A = \Delta P - \epsilon . \tag{34}$$

We record ϵ instead of adjusting the analyzer scale to make it zero as in reference 4.

For the alinement of the polarizer, a metal surface is used with the arms set for reflection at an angle near the principal angle. The analyzer is set with the plane of transmission approximately in the plane of the surface ($A_s \approx 90°$). As described in reference 4, the polarizer then is adjusted for minimum transmission ($P_s \approx 0°$) and the intensity of the minimum noted. A_s is moved by 0.1 degree and P_s is again adjusted for a minimum and the intensity noted. If the intensity has increased A_s is adjusted in the opposite direction. By taking a series of readings, setting the analyzer by increments, and adjusting the polarizer for a minimum, we can plot P_s versus A_s and determine the point on this curve which intersects the line $P_s = A_s - \epsilon - 90°$ which is also the line $P = A - 90°$.

We may also approach this point directly by using smaller and smaller increments of A_s in an attempt to find scale readings P_s and A_s such that

$$A_s - P_s = 90° + \epsilon \qquad (35)$$

within 0.01 degree. Thus, the point at which both $P = A - 90°$ and minimum transmission occur is obtained by setting A_s and adjusting P_s. This method has been shown to be the only unambiguous way of alining the ellipsometer [4]. At this point the plane of transmission of the polarizer is in the plane of incidence; therefore, $P = 0$ and, by eq 31, $\Delta P = -P_s$ and ΔP is determined. ΔA can then be calculated by eq 34.

The wave plate is alined by inserting it between crossed polarizer and analyzer in the straight through position with the polarizer set at zero ($P = 0°$, $A = 90°$ or $P_s = -\Delta P$, $A_s = 90° - \Delta A$) and adjusting it near the zero reading of the fast axis for minimum transmission. At this minimum the fast axis of the wave plate will be set to the azimuth of the polarizer which is zero. By eq 33,

$Q_s + \Delta Q = 0°$

$$\Delta Q = -Q_s . \qquad (36)$$

The three alinement corrections, ΔP, ΔA, and ΔQ, have now been obtained and may be used on the ALINE card as shown in table 2.

Appendix II

Derivation of Equation 3

The derivation uses Jones vector and matrices as described in "Polarized Light" by W. Shurcliff [15].

The normalized Jones vector of the light from the polarizer, expressed in x and y axes along the fast and slow axes of the wave plate, is $\begin{bmatrix} \cos{(P-Q)} \\ \sin{(P-Q)} \end{bmatrix}$ where P and Q are azimuths of the polarizer and fast axis of the wave plate measured from the plane of incidence of the reflection. The matrix for the wave plate is $\begin{bmatrix} 1 & 0 \\ 0 & \rho_c \end{bmatrix}$.

The light is now expressed with respect to x and y axes along and normal to the plane of incidence by use of the counter-rotator matrix $\begin{bmatrix} \cos Q & -\sin Q \\ \sin Q & \cos Q \end{bmatrix}$.

The matrix for reflection from the surface is simply $\begin{bmatrix} \rho & 0 \\ 0 & 1 \end{bmatrix}$.

Therefore, the light after reflection from the surface is given by

$$\begin{bmatrix} \rho & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \cos Q & -\sin Q \\ \sin Q & \cos Q \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \rho_c \end{bmatrix} \begin{bmatrix} \cos{(P-Q)} \\ \sin{(P-Q)} \end{bmatrix}$$

$$= \begin{bmatrix} \rho[\cos Q \cos{(P-Q)} - \rho_c \sin Q \sin{(P-Q)}] \\ \sin Q \cos{(P-Q)} + \rho_c \cos Q \sin{(P-Q)} \end{bmatrix}.$$

For this light to be extinguished by the analyzer, it must be linearly polarized. In this case, its azimuth e is given by

$$\tan e = \frac{\sin Q \cos{(P-Q)} + \rho_c \cos Q \sin{(P-Q)}}{\rho[\cos Q \cos{(P-Q)} - \rho_c \sin Q \sin{(P-Q)}]}$$

$$= \frac{\tan Q + \rho_c \tan{(P-Q)}}{\rho[1 - \rho_c \tan Q \tan{(P-Q)}]}.$$

The analyzer must be set 90° from e to extinguish the light so

$$\tan A = -1/\tan e \; ;$$

therefore,

$$\tan A = \frac{\rho[\rho_c \tan Q \tan (P-Q) -1]}{\tan Q + \rho_c \tan (P-Q)} \; .$$

Solving for ρ gives eq 3.

NM 1.

NF 1.4

NS 1.7

A1 65.

CTABLE 0.   20.   1.08000   100.

INDEX OF MEDIUM= 0.   1.08000   20.   1.00000   ANGLE OF INCIDENCE= 65.000   WAVE LENGTH= 5461.00   TC= 1.00000   DELC= 90.000

THICK	DEL	PSI	RF.CF.PARRALLEL		RF.CF.NORMAL		NF	KAPPA	NS	KAPPA	P1	A1	P2	A2
.0	.000	8.498	.08155	180.000	.54579	180.000	1.4000	-.0000	1.7000	-.0000				
20.0	2.087	8.508	.08164	-178.462	.54570	179.452	1.4000	-.0000	1.7000	-.0000				
40.0	4.161	8.538	.08189	-176.935	.54544	178.904	1.4000	-.0000	1.7000	-.0000				
60.0	6.211	8.588	.08230	-175.433	.54500	178.356	1.4000	-.0000	1.7000	-.0000				
80.0	8.224	8.657	.08288	-173.966	.54438	177.810	1.4000	-.0000	1.7000	-.0000				
100.0	10.191	8.744	.08361	-172.544	.54359	177.264	1.4000	-.0000	1.7000	-.0000				

THICK	DEL	PSI	RF.CF.PARRALLEL		RF.CF.NORMAL		NF	KAPPA	NS	KAPPA	P1	A1	P2	A2
.0	.000	8.498	.08155	180.000	.54579	180.000	1.5000	-.0000	1.7000	-.0000				
20.0	1.629	8.507	.08162	-178.748	.54571	179.623	1.5000	-.0000	1.7000	-.0000				
40.0	3.247	8.531	.08183	-177.507	.54547	179.246	1.5000	-.0000	1.7000	-.0000				
60.0	4.846	8.573	.08217	-176.284	.54508	178.870	1.5000	-.0000	1.7000	-.0000				
80.0	6.416	8.630	.08264	-175.088	.54453	178.496	1.5000	-.0000	1.7000	-.0000				
100.0	7.947	8.703	.08325	-173.929	.54382	178.124	1.5000	-.0000	1.7000	-.0000				

CTABLE 0.   100.   45.

INDEX OF MEDIUM= 0.   1.00000   100.   1.00000   ANGLE OF INCIDENCE= 65.000   WAVE LENGTH= 5461.00   TC= 1.00000   DELC= 90.000

THICK	DEL	PSI	RF.CF.PARRALLEL		RF.CF.NORMAL		NF	KAPPA	NS	KAPPA	P1	A1	P2	A2
.0	.000	8.498	.08155	180.000	.54579	180.000	1.4000	-.0000	1.7000	-.0000	135.00	8.50	45.00	171.50
20.0	2.087	8.508	.08164	-178.462	.54570	179.452	1.4000	-.0000	1.7000	-.0000	133.96	8.51	43.96	171.49
40.0	4.161	8.538	.08189	-176.935	.54544	178.904	1.4000	-.0000	1.7000	-.0000	132.92	8.54	42.92	171.46
60.0	6.211	8.588	.08230	-175.433	.54500	178.356	1.4000	-.0000	1.7000	-.0000	131.89	8.59	41.89	171.41
80.0	8.224	8.657	.08288	-173.966	.54438	177.810	1.4000	-.0000	1.7000	-.0000	130.89	8.66	40.89	171.34
100.0	10.191	8.744	.08361	-172.544	.54359	177.264	1.4000	-.0000	1.7000	-.0000	129.90	8.74	39.90	171.26

THICK	DEL	PSI	RF.CF.PARRALLEL		RF.CF.NORMAL		NF	KAPPA	NS	KAPPA	P1	A1	P2	A2
.0	.000	8.498	.08155	180.000	.54579	180.000	1.5000	-.0000	1.7000	-.0000	135.00	8.50	45.00	171.50
20.0	1.629	8.507	.08162	-178.748	.54571	179.623	1.5000	-.0000	1.7000	-.0000	134.19	8.51	44.19	171.49
40.0	3.247	8.531	.08183	-177.507	.54547	179.246	1.5000	-.0000	1.7000	-.0000	133.38	8.53	43.38	171.47
60.0	4.846	8.573	.08217	-176.284	.54508	178.870	1.5000	-.0000	1.7000	-.0000	132.58	8.57	42.58	171.43
80.0	6.416	8.630	.08264	-175.088	.54453	178.496	1.5000	-.0000	1.7000	-.0000	131.79	8.63	41.79	171.37
100.0	7.947	8.703	.08325	-173.929	.54382	178.124	1.5000	-.0000	1.7000	-.0000	131.03	8.70	41.03	171.30

Figure 1. Instruction CTABLE.

NM 1.33

NF 2.5

AI 65.

CNS 86.35 25.19 176.35 154.81 45.

DEL1= 86.350 25.190 176.350 154.810 45.000
       97.300003 PSI1= 25.189998 DEL2= 97.300007 PSI2= 25.190002
DEL=   97.300006 PSI1= 25.189999

INDEX OF SUBSTRATE= 2.0000   DEL= 1.0002   DEL= 97.300 PSI= 25.190

CD 94.30 24.44 45.
    94.300 24.440 45.000
DEL= 81.400000 PSI= 24.439999

INDEX OF MEDIUM= 1.33000 ANGLE OF INCIDENCE= 65.000 WAVE LENGTH= 5461.00 TC= 1.00000 DELC= 90.000

THICK	N2 REAL	KAPPA	ADSORPTION	Δ DEL	Δ PSI	ERROR	N2-N1	N3-N2 WT FRACTION	NS REAL	KAPPA	K 2
100.6	2.50000	.30000	4.8265-03	-.009	.023	-.38856	1.17000	-.50005 4.79826	1.99995	1.00016	2

Figure 2. Instructions CNS and CD.

AI 60.

WL 5893.

NS 1.51163

NF 1.1 .25 1.5

CND 16.943 11.856

INDEX OF MEDIUM= 1.00000 ANGLE OF INCIDENCE= 60.000 WAVE LENGTH= 5893.00 TC= 1.00000 DELC= 90.000

THICK	N2 REAL	KAPPA	ADSORPTION	Δ DEL	Δ PSI	ERROR	N2-N1	N3-N2 WT FRACTION	NS REAL	KAPPA	K 2
1000.0	1.40000	.00000	8.2425-03	-.001	-.000	.01848	.40000	.11630 .82425	1.51630	.00000	2

Figure 3. Instruction CND.

```
AI    60.

WL    5893.

NS    1.5163

NF    1.1    .25    1.5

EDP   .1    .1

CNDC  16.943    11.856
```

INDEX OF MEDIUM= 1.00000 ANGLE OF INCIDENCE= 60.000 WAVE LENGTH= 5893.00 TC= 1.00000 DELC= 90.000

THICK	N2 REAL	KAPPA	ADSORPTION	Δ DEL	Δ PSI	ERROR	N2-N1	N3-N2	WT FRACTION	NS REAL	KAPPA	K
1000.0	1.40000	.00000	8.2425-03	-.001	-.000	.01848	.40000	.11630	.82425	1.51630	.00000	2
998.0	1.39974	.00000	8.2213-03	-.000	-.000	.01110	.39974	.11656	.82378	1.51630	.00000	2
1002.0	1.40026	.00000	8.2638-03	-.001	-.000	.03863	.40026	.11604	.82472	1.51630	.00000	2
1005.9	1.39861	.00000	8.2655-03	-.001	-.000	.02176	.39861	.11769	.82172	1.51630	.00000	2
994.0	1.40139	.00000	8.2182-03	.001	.000	-.02374	.40139	.11491	.82678	1.51630	.00000	2
1002.8	1.39883	.00000	8.2437-03	.002	.000	-.04887	.39883	.11747	.82211	1.51630	.00000	2
1005.6	1.39919	.00000	8.2736-03	.001	.000	-.01686	.39919	.11711	.82277	1.51630	.00000	2
994.3	1.40080	.00000	8.2102-03	.001	.000	-.03461	.40080	.11550	.82569	1.51630	.00000	2
997.2	1.40116	.00000	8.2404-03	.001	.000	-.03520	.40116	.11514	.82636	1.51630	.00000	2

CONFIDENCE LIMITS OF FILM THICKNESS IS 994.0 TO 1005.9
CONFIDENCE LIMITS OF THE REAL PART OF INDEX OF REFRACTION OF FILM IS 1.39861 TO 1.40139

```
CNDE  16.943    11.856
```

INDEX OF MEDIUM= 1.00000 ANGLE OF INCIDENCE= 60.000 WAVE LENGTH= 5893.00 TC= 1.00000 DELC= 90.000

THICK	N2 REAL	KAPPA	ADSORPTION	Δ DEL	Δ PSI	ERROR	N2-N1	N3-N2	WT FRACTION	NS REAL	KAPPA	K
1000.0	1.40000	.00000	8.2425-03	-.001	-.000	.01848	.40000	.11630	.82425	1.51630	.00000	2

CONFIDENCE LIMITS OF FILM THICKNESS IS 994.0 TO 1005.9
CONFIDENCE LIMITS OF THE REAL PART OF INDEX OF REFRACTION OF FILM IS 1.39861 TO 1.40139

Figure 4. Instructions CNDC and CNDE.
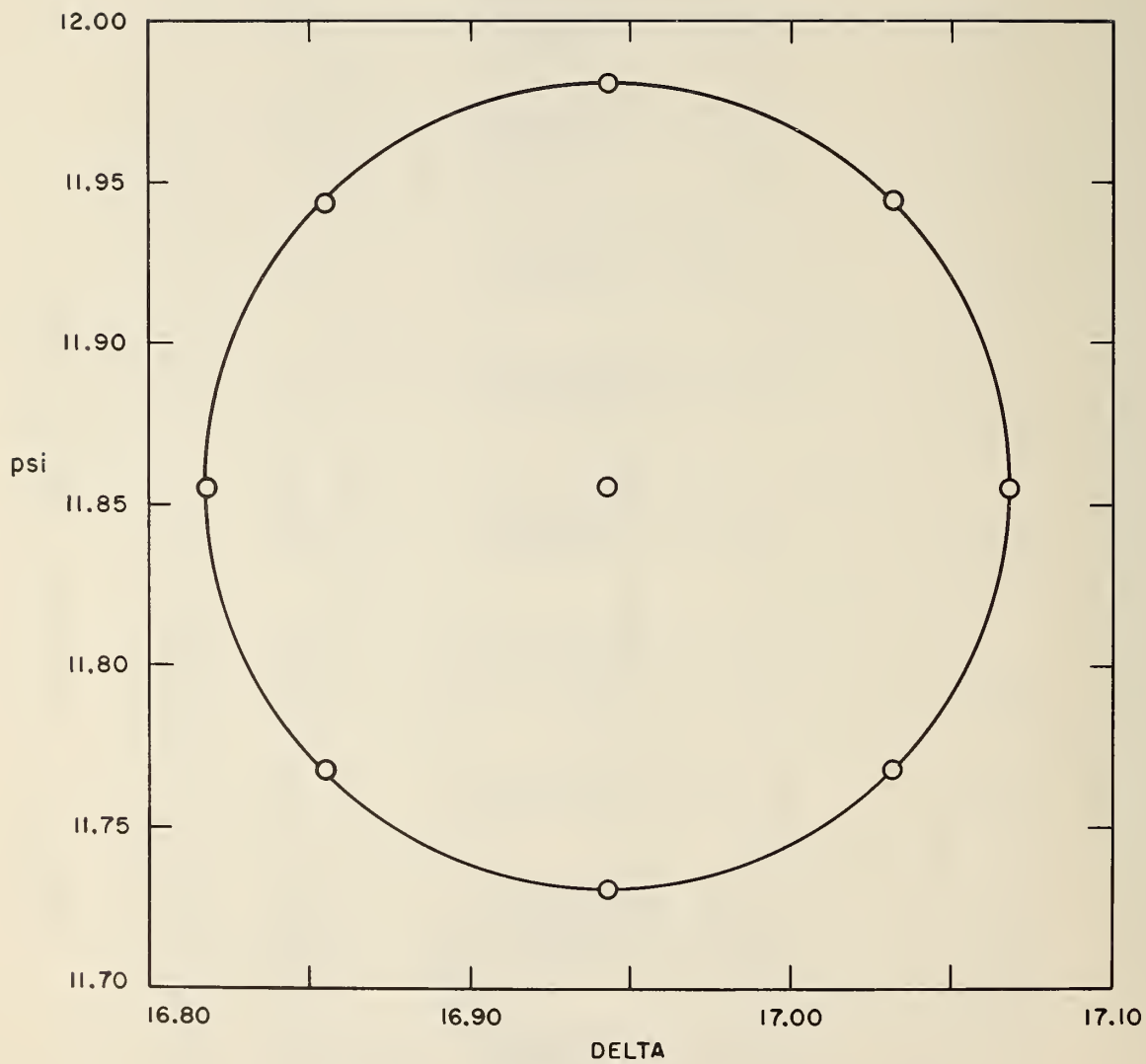
Figure 5. Confidence ellipse for measurements Δ and ψ .
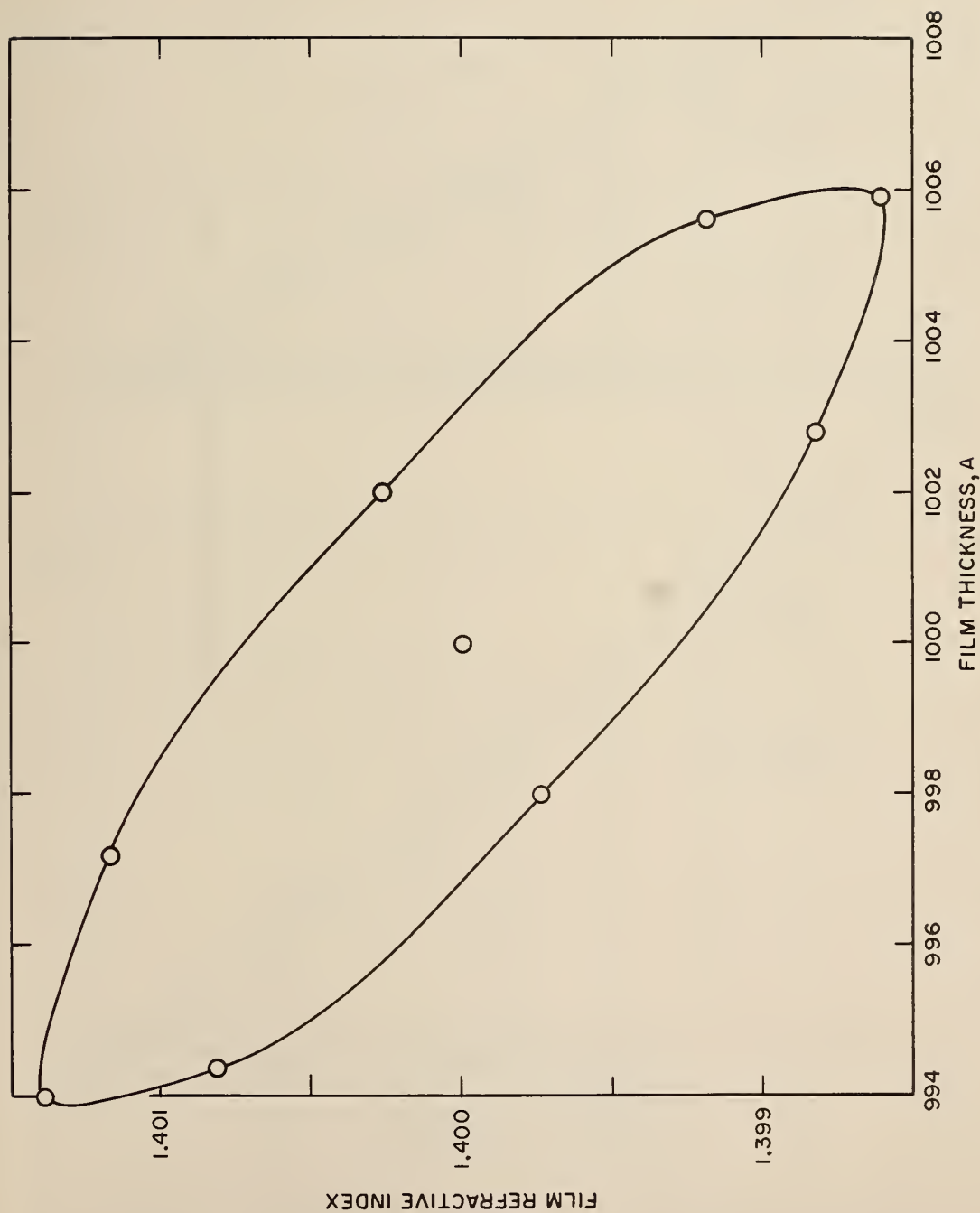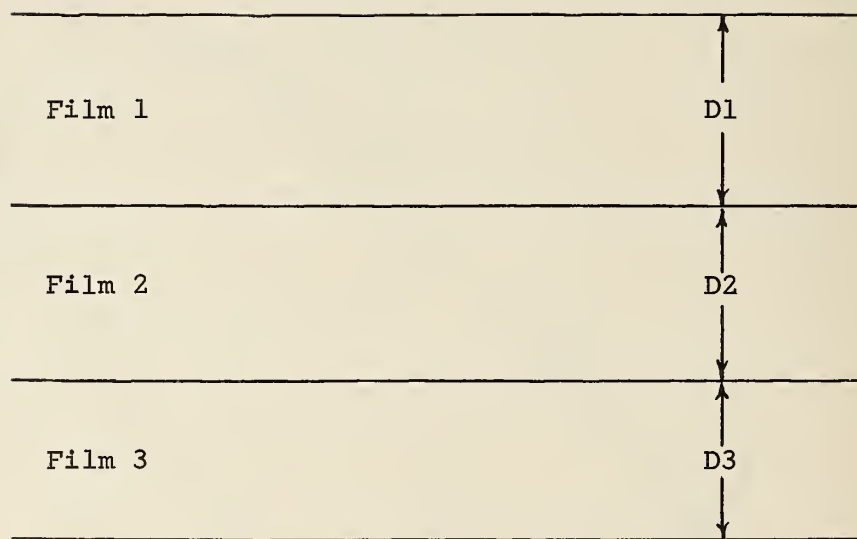
Figure 6. Confidence ellipse for calculated values of the refractive index and thickness of the film.

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Surrounding
 Medium

Film 1   D1

Film 2   D2

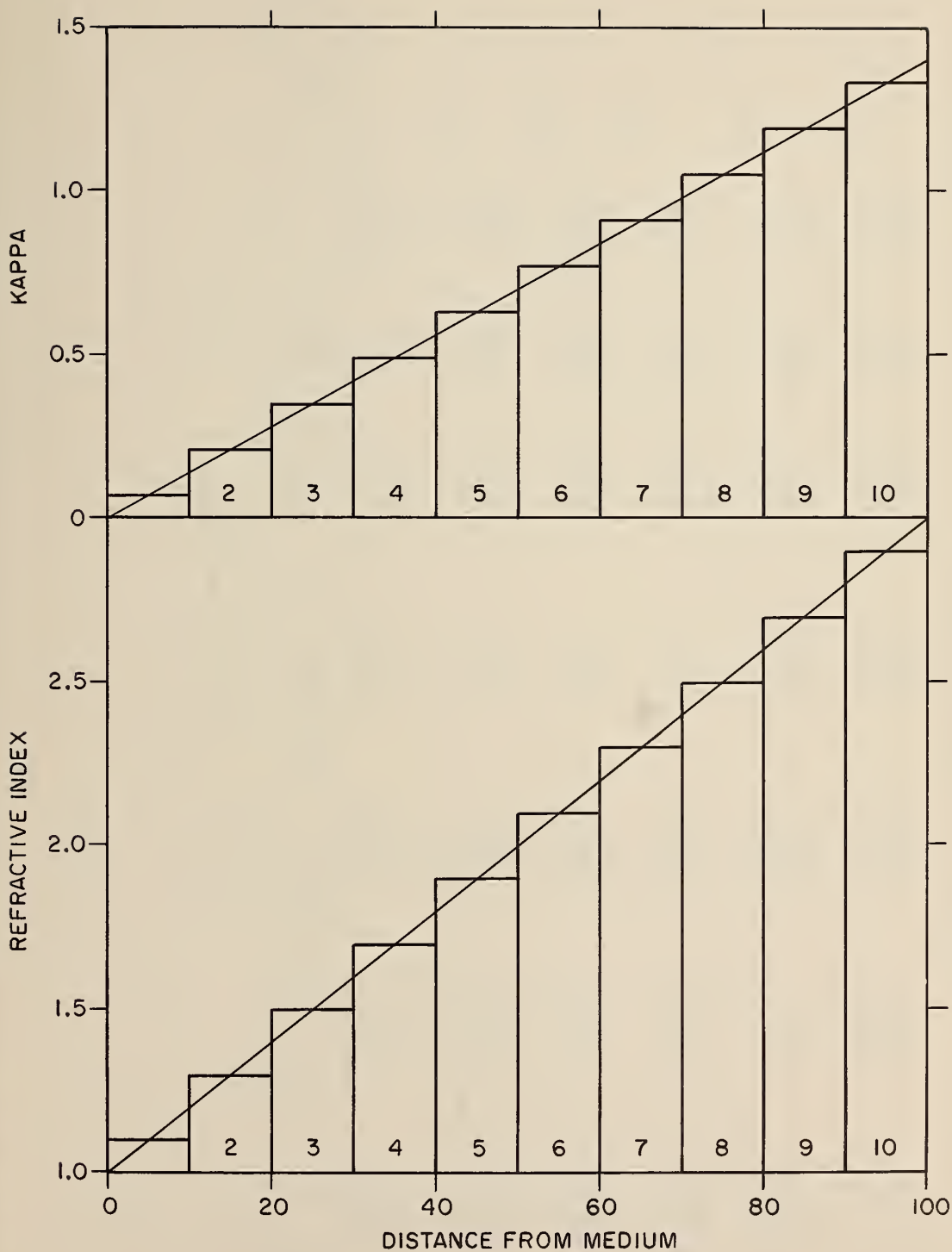Film 3   D3

Substrate

Fig. 7. . - Schematic diagram of three films on a
           Substrate.

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Figure 8.   Approximation of an inhomogeneous film by ten
homogeneous films.

```
NS     3.

NF     1.1                    1.4
                              .07
FILM   2.    10.    1.3       .21
FILM   3.    10.    1.5       .35
FILM   4.    10.    1.7       .49
FILM   5.    10.    1.9       .63
FILM   6.    10.    2.1       .77
FILM   7.    10.    2.3       .91
FILM   8.    10.    2.5      1.05
FILM   9.    10.    2.7      1.19
FILM  10.    10.    2.9      1.33

CTABLE 10.

INDEX OF MEDIUM=  1.00000   ANGLE OF INCIDENCE=  70.000   WAVE LENGTH=  5461.00   TC=  1.00000   DELC=  90.000

                RF.CF.NORMAL       NF      KAPPA      NS     KAPPA      P1      A1      P2      A2
                .92027 170.656   1.1000    .0700    3.0000   1.4000

  THICK    DEL      PSI     RF.CF.PARRALLEL     RF.CF.NORMAL
  10.0   117.558  30.841     .54949 -71.786      .92027 170.656
```

Figure 9. Instruction FILM.

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```
NS    4.05                            .00741

FT    1600.    100.    2100.

NF    1.    .2    4.                  0.    .02    .5

CNK   104.57   13.28

INDEX OF MEDIUM= 1.00000   ANGLE OF INCIDENCE= 70.000   WAVE LENGTH= 5461.00   TC= 1.00000   DELC= 90.000
```

NF	KAPPA	ΔNF	ΔKAPPA	ERROR	ΔDELTA	ΔPSI	THICK
1.02480	.04414	.00010	.00001	.00031	-.077	-.060	1600.0
2.18437	.02486	.00010	.00001	.00004	-.007	.001	
2.75254	.43270	.00010	.00001	.00001	.008	.001	
1.02148	.04283	.00010	.00001	.00008	.037	.045	1700.0
2.06133	.02652	.00010	.00001	.00002	-.001	.000	
2.74902	.43605	.00010	.00001	.00002	.006	.001	
1.01836	.04160	.00010	.00001	.00039	-.114	-.070	1800.0
1.95781	.02693	.00010	.00001	.00009	-.019	.004	
2.74395	.43807	.00010	.00001	.00001	-.012	-.000	
1.01563	.04037	.00010	.00001	.00010	.063	.050	1900.0
1.86934	.02676	.00010	.00001	.00004	-.015	.003	
2.73945	.43881	.00010	.00001	.00001	-.012	.000	
1.01309	.03918	.00010	.00001	.00007	-.125	-.056	2000.0
1.79297	.02629	.00010	.00001	.00014	-.012	.003	
2.73672	.43859	.00010	.00001	.00001	-.006	-.000	
1.01074	.03803	.00010	.00001	.00012	-.147	-.064	2100.0
1.72617	.02568	.00010	.00001	.00003	-.010	.004	
2.73555	.43793	.00010	.00001	.00001	.011	-.000	

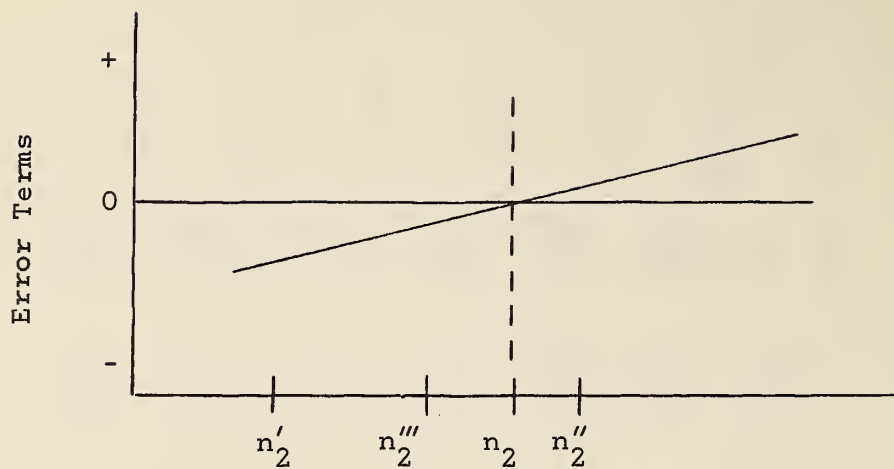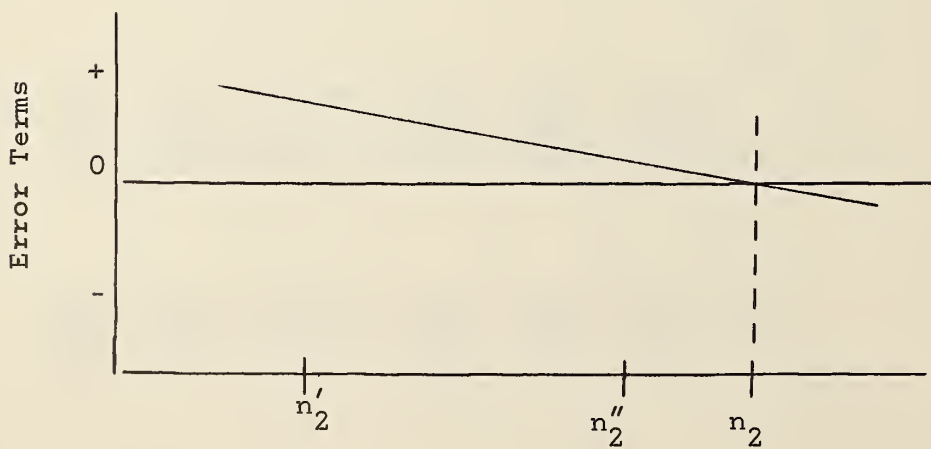Figure 10.   Instructions CNK and FT.

Figure 11a.   Refractive index of film.

Figure 11b.   Refractive index of film.
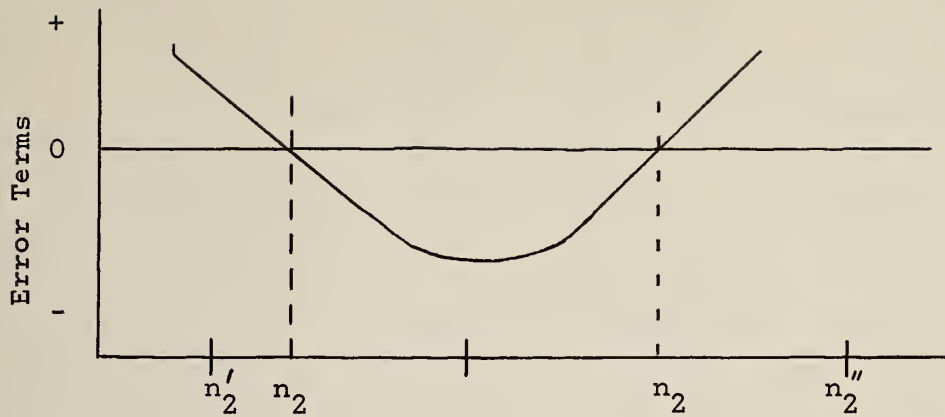
Figure 11c.   Refractive index of film.

Figure 11d.   Refractive index of film.

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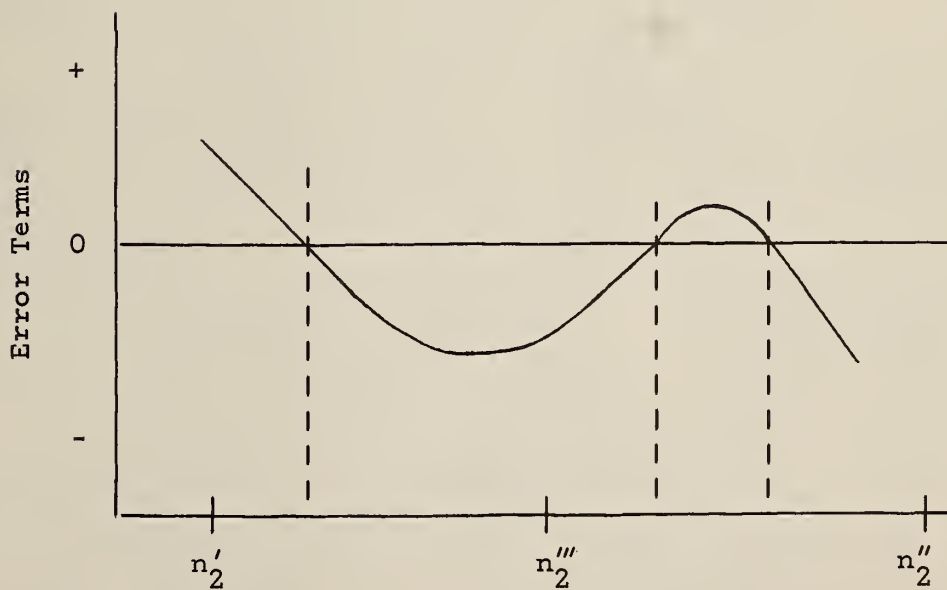
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